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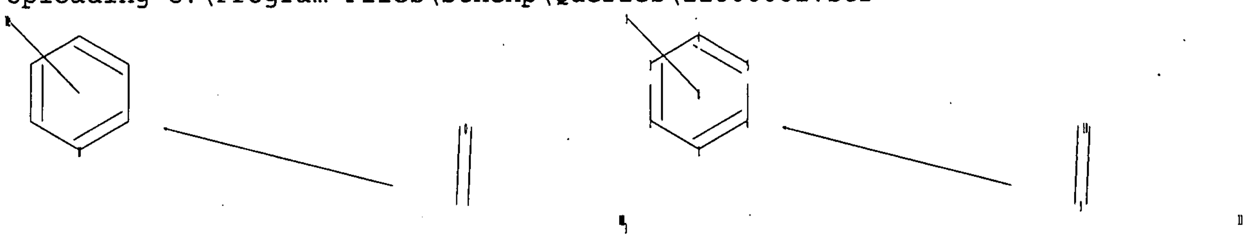


chain nodes :
7 9 10 11
ring nodes :
1 2 3 4 5 6
chain bonds :
9-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
9-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:CLASS 10:CLASS
11:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 9
containing 11

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR

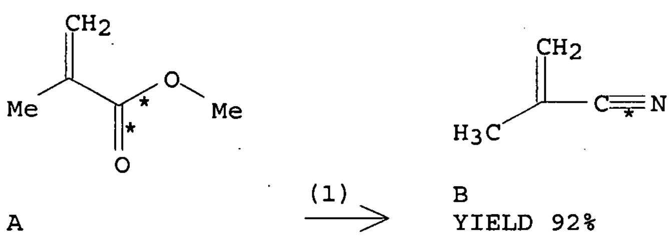
ACCESSION NUMBER: 137:247610 CASREACT <<LOGINID::20070611>>
TITLE: Preparation of nitriles from esters
INVENTOR(S): Koji, Takayuki; Miura, Hiroshi; Nishimoto, Yoshihiro
PATENT ASSIGNEE(S): Koei Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002284753	A	20021003	JP 2001-85177	20010323

PRIORITY APPLN. INFO.: JP 2001-85177 20010323

AB Nitriles are prepared by reaction of carboxylic acid esters with ammonia in the presence of titania or zirconia. Thus, reaction of Me methacrylate with ammonia in the presence of titania at 300° gave 92.6% methacrylonitrile.

RX(1) OF 2 A ===> B



A (1) B
YIELD 92%

RX(1) RCT A 80-62-6
RGT C 7664-41-7 NH_3
PRO B 126-98-7
CAT 13463-67-7 TiO_2
NTE gas phase

A novel single step synthesis of 2-methyl-6-phenylpyridine from non-heterocyclic compounds over molecular sieve catalysts†

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The industrially important 2-methyl-6-phenylpyridine is synthesized for the first time in a single step by reacting acetophenone, acetone, formaldehyde and ammonia in the vapor phase over microporous and mesoporous molecular sieve catalysts.

Introduction

Conventional homogeneous acid catalysts such as H_2SO_4, HF, $AlCl_3$, $FeCl_3$ *etc.*, show several disadvantages such as high corrosiveness, tedious work-up, requirement of stoichiometric quantities, the presence of several undesirable side products, and non-recycling of catalyst, and thus are highly non-ecofriendly. The major goals of 'Green chemistry' are to increase process selectivity, maximize the use of starting materials, and to replace hazardous and stoichiometric reagents with eco-friendly catalysts in order to facilitate easy separation of the final reaction mixture, including recovery of the catalyst. Microporous aluminosilicate molecular sieves have been studied extensively in the area of acid catalysis and cyclization reactions, and these materials have contributed greatly to hydrocarbon processing and the chemical industry.[1] Mesoporous MCM-41 materials have well defined pore sizes of 15–100 Å, *i.e.* larger than the pore size constraint of 15 Å) characteristic of microporous zeolites. The large pore size (relative to that of microporous zeolites) reduces diffusional restriction of reactants and products and so enables reactions involving bulky molecules to occur.[2–4] Although extensive research efforts have been undertaken to explore the catalytic applications of modified MCM-41 materials in the field of catalytic oxidations,[5,6] acid catalysis[7] and alkylation reactions[8] applications in a variety of fields of organic chemistry still remain limited.

Among heterocyclic compounds, alkyl substituted phenylpyridines are extensively used as intermediates in the synthesis of drugs, pharmaceuticals, herbicides and agrochemicals.[9] A substituted phenylpyridine 2-(4-carboxyphenyl)pyridine is a starting material for BMS-232632, a potent azapeptide HIV protease inhibitor which has shown high anti-HIV activity.[10] Among various synthetic routes for pyridine and its derivatives, aldehyde/ketone and ammonia condensation is a commercially proven success.

The synthesis of 2-methyl-6-phenylpyridine over molecular sieve catalysts has not been reported. 2-Phenylpyridine and substituted 2-phenylpyridines are generally synthesized from the reaction of aryllithium with pyridine and picolines in homogenous conditions.[11] Regioselective alkylation of 2-phenylpyridine with olefins in the presence of Rh(I) as a catalyst gave 3-methyl-2-phenylpyridine[12] and 2-(4-methylphenyl)pyridine,[13] but not 2-methyl-6-phenylpyridine. It was reported that 2-methyl-6-phenylpyridine can be synthesized by a homogeneous photocatalytic reaction from benzonitrile and ethylene using a Co(I) complex as a photocatalyst.[14] A Japanese patent[9] reported that acetophenones catalytically react with symmetric ketones, formaldehyde and ammonia using a metal-modified amorphous silica-alumina catalyst in the vapor phase at 350–550 °C, however, the amorphous silica-alumina catalyst is prone to deactivation with time on stream.

Here, we report for the first time, the synthesis of 2-methyl-6-phenylpyridine over a novel mesoporous MCM-41 catalyst in a continuous fixed bed using simple and inexpensive raw materials, *i.e.* acetophenone, acetone, formaldehyde and ammonia.

Results and discussion

The heterocyclization reaction of acetophenone, acetone, formaldehyde and ammonia for the synthesis of 2-methyl-6-phenylpyridine was carried out over HZSM-5, HM, Hβ, HY and MCM-41 catalysts and the results are shown in Table 1 and in Fig. 1. The order of catalytic activity for 2-methyl-6-phenylpyridine was found to be MCM-41 > HY > Hβ > HM ⩾ HZSM-5. It is assumed that the small pore size (5.4 Å) of the HZSM-5 zeolites imposes diffusion control through which the bulky product 2-methyl-6-phenylpyridine can not diffuse out, with the formation of the small amount of the product probably through a surface reaction. The intermediate activity of HY zeolite (pore size 7.4 Å) indicates that diffusion control is reduced compared to HZSM-5 for the large size product 2-methyl-6-phenylpyridine. The lowerer catalytic activity of Hβ relative to HY may be due to its geometry of two

Green Context

The ability to carry out clean synthetic transformations over solid catalysts has been transformed by the advent of MCM type materials. While initial attempts to use the larger pores showed that the acidity of the materials is much lower than that of most zeolites of similar composition, this can often be advantageous. Here, for example, a multicomponent condensation is carried out using the large pore dimensions and mild acidity of these materials. It is shown that yields of this gas phase (no-solvent) reaction are much better than found with a range of zeolites. ***DJM***

† IICT Communication No. 4649.

DOI: 10.1039/b008914l

types of pores (pore sizes: 5.4 and 7.6 Å) in the intersecting channel system. It is observed that mesoporous Al-MCM-41 (pore size 30 Å) shows high catalytic activity for 2-methyl-6-phenylpyridine formation with no diffusional constraint. It is evident from the data shown in Fig. 1 that the pore size of the catalyst plays a major role during the synthesis of 2-methyl-6-phenylpyridine, a large molecule. Fig. 1 summarizes the important relation between pore size and molecular size of the reactant/product. The pore size of the catalyst must be accessible to reactant and product molecules in order to take part in the reaction.

A plausible reaction mechanism based on the product distribution is given in Scheme 1, which involves a multi-reactant system leading to several competitive and parallel reactions. Acetophenone and acetone upon reacting with ammonia form the corresponding imines. Thus, the two molecules of imine which form react with formaldehyde and subsequently undergo cyclization and dehydrogenation reactions leading to the formation of 2-methyl-6-phenylpyridine. Similarly, cyclization between two imine molecules of acetone and formaldehyde resulted the formation of 2,6-lutidine as a major side product. In similar manner, the reaction between two molecules of imine deriving from acetophenone and formal-

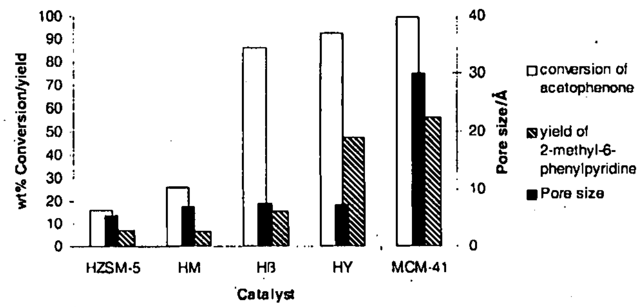
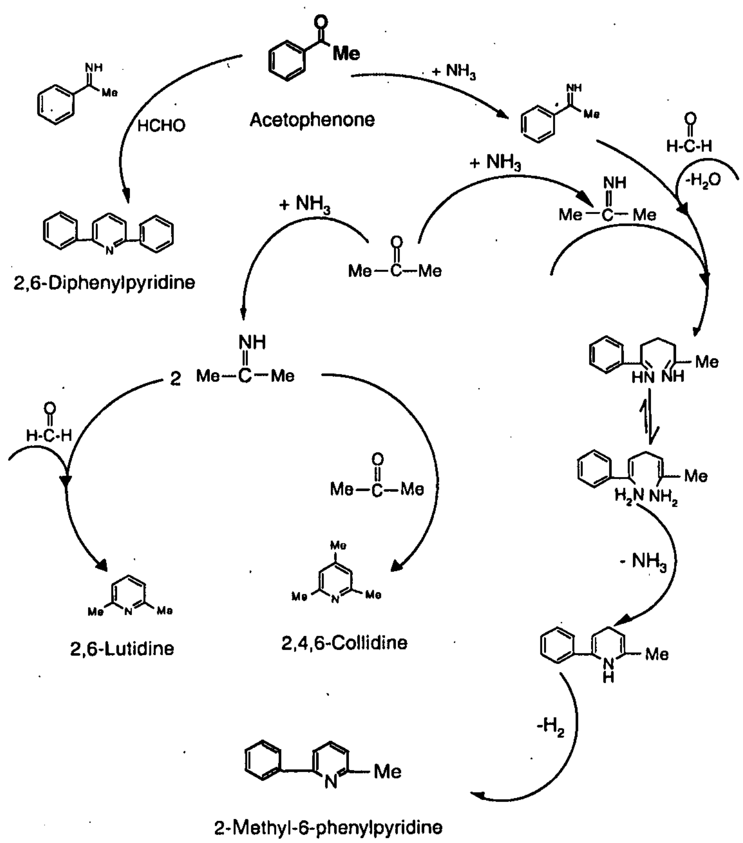


Fig. 1 Effect of pore size on the synthesis of 2-methyl-6-phenylpyridine.

Table 1 Synthesis of 2-methyl-6-phenylpyridine over molecular sieve catalysts

Catalyst	SiO_2/Al_2O_3	TOS/h	Conversion of acetophenone (wt%)	Yield of 2-methyl-6-phenylpyridine (wt%)[a]	Pore size/Å
HZSM-5	30	1	50.6	15.7	5.4
		4	16.0	7.2	
HM		4	25.9	6.3	7.1
Hβ	20	1	83.0	28.0	7.6, 5.4
		4	86.2	15.6	
HY	2.9	1	99.1	48.0	7.4
		4	92.3	47.5	
MCM-41	25	3	99.4	58.6	30
		4	99.3	56.0	
SiO_2-Al_2O_3	4	4	86.1	21.5	—
		4	86.1	21.5	—

Feed = acetophenone : acetone : formaldehyde : ammonia = 1 : 1.5 : 1 : 5 (molar ratio); reaction temperature = 400 °C; weight hour space velocity (WHSV) = 0.5 h^{-1}. [a] The yields are calculated based on the acetophenone conversion.



Scheme 1 A plausible reaction mechanism for the formation of various products during the synthesis of 2-methyl-6-phenylpyridine.

dehyde lead to the formation of 2,6-diphenylpyridine. Furthermore, 2- and 4-picolines were observed as minor products. The isomers of alkylated and mono- and di-methyl- phenylpyridines result from the cyclization of acetone with acetophenone in different mol ratios in the presence of formaldehyde and ammonia. Aldol condensation products of acetophenone and acetone are also observed in trace amounts. Ethylbenzene, trace amounts of styrene, α-methylstyrene and cumene were also observed. The internal acidity of the zeolites is responsible for the various transformations. It is clear that the acidic strength of the sites depends on the chemical composition of the zeolite and is related to the framework topology. It was observed that medium strength acid sites are favored for the required specific heterocyclization product.

Conclusion

In conclusion, this work shows that mesoporous molecular sieves such as MCM-41 are active catalysts for heterocyclization reactions, especially in the present case, for the synthesis of 2-methyl-6-phenylpyridine. It is also shown that the large pore mesoporous MCM-41 catalyst is more active than microporous aluminosilicates like HZSM-5, HM, Hβ and HY zeolites for the synthesis of 2-methyl-6-phenylpyridine which is a large molecule. The data also substantiate the phenomenon of diffusion control of reactants, products and shape selectivity with respect to pore size of the catalysts.

Experimental

Al-MCM-41 was prepared as reported by Ortlam *et al.*[15] and calcined at 500 °C in air for 12 h. The BET surface area was determined by N_2 adsorption at 77 K and also characterized by XRD, IR and MAS-NMR spectroscopic techniques. The HZSM-5 zeolite was obtained from Conteka (Sweden), Hβ was obtained from Sud-chemie (India) and HM, HY zeolites were obtained from PQ Corporation (USA).

The cyclization reaction was carried out in a continuous fixed-bed down-flow Pyrex glass reactor of internal diameter 18 mm, using 4 g of the sized catalyst (18–30 mesh) in the middle of the reactor, with an electrically heated furnace. The reaction was carried out at 400 °C. The feed (acetophenone: acetone: formaldehyde: ammonia = 1 : 1.5 : 1 : 5 mol ratio) was fed from the top of the reactor using a B. Braun (Germany) syringe pump. The products were collected through an ice-cold water trap and analyzed by GC (10% SE-30, 20 % Carbowax in 1.8 meter S.S. packed columns) and identified by GC–MS and ^{1}H NMR spectroscopy.

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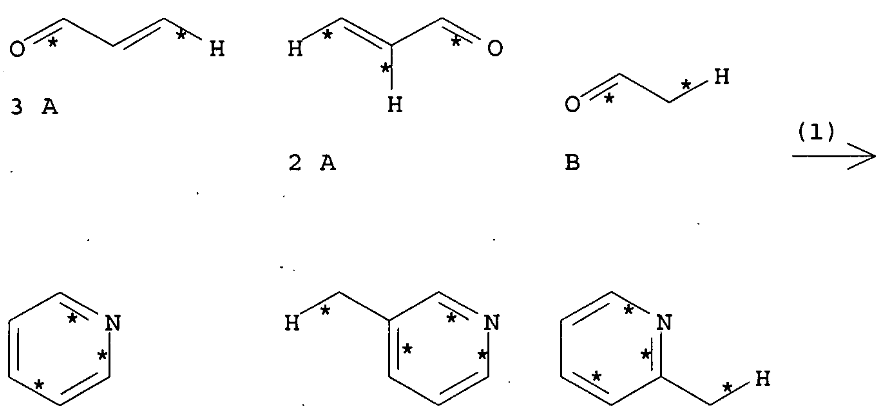
ACCESSION NUMBER: 126:89276 CASREACT <<LOGINID::20070611>>
TITLE: Preparation of pyridine bases by catalytic gas -phase reaction of aldehydes and/or ketones with ammonia
PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08333343	A	19961217	JP 1996-142175	19960513
EP 764638	A1	19970326	EP 1996-401325	19960618
EP 764638	B1	20010418		
R: BE, DE, FR, GB, IT, NL				
PRIORITY APPLN. INFO.:			US 1995-481082	19950607
			JP 1995-270607	19950925
			JP 1996-142175	19960513

AB Claimed is a process for preparation of the title compds. by gas-phase cyclocondensation of aldehydes and/or ketones with ammonia over metal-zeolite catalysts. The title compds., useful as intermediates in the production of drugs and pesticides, are prepared in an industrial manner safely and economically. Thus, a mixture of CH2:CHCHO, MeCHO, and NH3 was reacted over HZSM-5/Ag (preparation given) at 450° for 6 h to give 45% pyridine, 27% β-picoline, and 1% α-picoline.

RX(1) OF 1 5 A + B ===> C + D + E



C
YIELD 45%

D
YIELD 27%

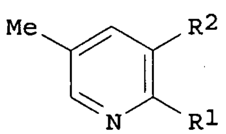
E
YIELD 1%

RX(1) RCT A 107-02-8, B 75-07-0
RGT F 7664-41-7 NH3
PRO C 110-86-1, D 108-99-6, E 109-06-8
CAT 7761-88-8 AgNO3
NTE 450.DEGREE. FOR 6 H; GHSV 500, HZSM-5 ALSO PRESENT AS CATALYST

ACCESSION NUMBER: 126:47101 CASREACT <<LOGINID::20070611>>
TITLE: Preparation of 3-methylpyridine derivatives by gas-phase catalytic cyclocondensation of methacrolein with carbonyl compounds and ammonia
INVENTOR(S): Uchiumi, Hiroshi; Anzai, Ryuichi
PATENT ASSIGNEE(S): Nitto Chemical Industry Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08259537	A	19961008	JP 1995-90099	19950324

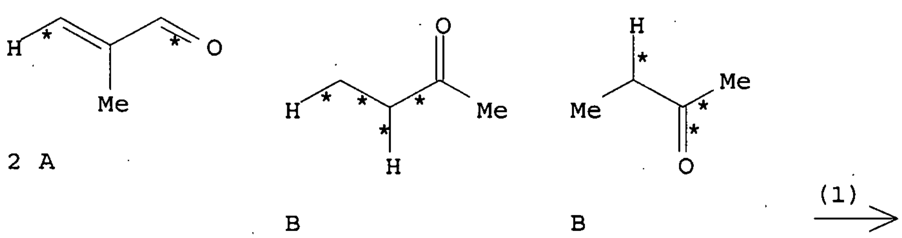
PRIORITY APPLN. INFO.: JP 1995-90099 19950324
OTHER SOURCE(S): MARPAT 126:47101
GI

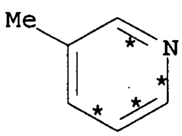


I

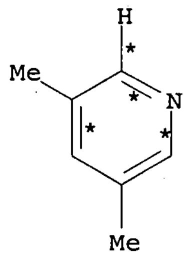
AB The title compds. (I; R1, R2 = H, C1-4 alkyl) are prepared by cyclocondensation of methacrolein with R1COCH2R2 (R1, R2 = same as above) and NH3 over catalysts SiaXbYcZdOe (X = P, B; Y = Li, Na, K, Rb, Cs, Mg, Sr, Ba, La; Z = Ce, Ti, Zr, V, Nb, etc.; a, b, c, d, e = atomic ratio; when a = 10, b = 0.2-10, c = 0-3, d = 0-5; e = number of corresponding to the formed oxide) in the presence of water steam. I are useful materials in the production of drugs, pesticides, and polymers. Thus, methacrolein was reacted with NH3 and MeCOEt over catalyst Si10P1.25B1.5O25.38 (preparation given) at 350° for 4.0 s. to give 22% I (R1 = R2 = Me) and 20% I (R1 = H, R2 = Me) resp.

RX(1) OF 1 2 A + 2 B ===> C + D





C
YIELD 22%



D
YIELD 20%

RX(1)

RCT A 78-85-3, B 78-93-3
RGT E 7664-41-7 NH3
PRO C 108-99-6, D 591-22-0
CAT 184580-39-0 Silicon borate oxide phosphate ($Si_{10}(BO_3)_{1.5}O_{15.88}(PO_4)_{1.25}$)
NTE 350° for 4 s

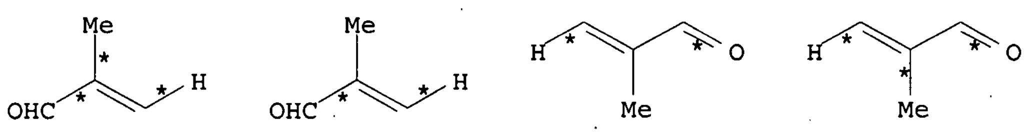
ACCESSION NUMBER: 126:18794 CASREACT <<LOGINID::20070611>>
TITLE: Preparation of di- and trimethylpyridine using silicon-containing metal oxide as catalysts
INVENTOR(S): Uchiumi, Hiroshi; Anzai, Ryuichi; Morya, Kyoshi
PATENT ASSIGNEE(S): Nitto Chemical Industry Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08245589	A	19960924	JP 1995-83488	19950316

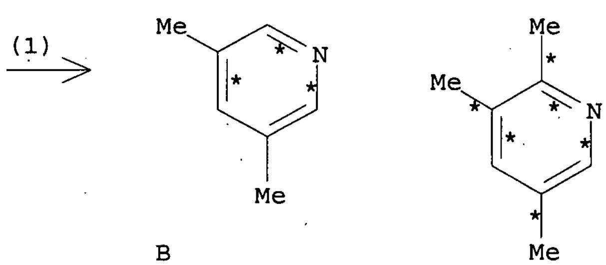
PRIORITY APPLN. INFO.: JP 1995-83488 19950316

AB The title compds. (I) are prepared by vapor-phase reaction of methacrolein with NH3 over catalysts SiaXbBcYdZeOf (X = Zr, Al, P; Y = Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba, La; Z = Ce, Ti, V, Nb, Ta, Cr, Mo, W, Mn, Re, Fe, Co, Ni, Cu, Ag, Zn, Sn, Pb, Sb, Bi, S, Te; a, b, c, d, e, f = atomic ratio; when a = 10, b = 0.2-25, c = 0-7, d = 0-3, e = 0-3; f = number of oxide) in the presence of water steam. I are useful materials in the production of drugs, pesticides, and polymers. Thus, methacrolein was reacted with NH3 over Si10P1.0B1.0O24 catalyst (preparation given) at 340 ° for 4.0 h to give 49.1% 3,5-di- and 6.9% 2,3,5-trimethylpyridine.

RX(1) OF 1 4 A ===> B + C



A A A A

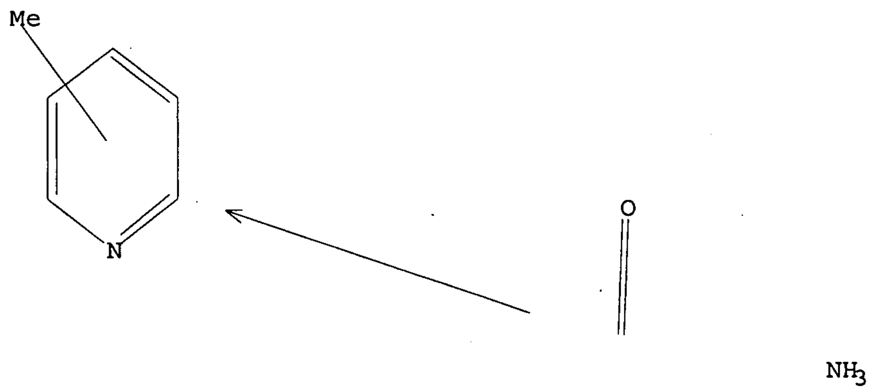


B
YIELD 49%

C
YIELD 7%

RX(1) RCT A 78-85-3
RGT D 7664-41-7 NH3
PRO B 591-22-0, C 695-98-7
CAT 184375-87-9 Silicon borate oxide phosphate (Si10(BO3)O17(PO4))

NTE 340° for 4 h; ratio of 17 : 9058 : N2 : H2O = 1 : 1 : 9 : 2; 100% convension



Structure attributes must be viewed using STN Express query preparation.

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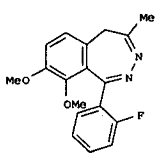
L2 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 146:229312 CASREACT
TITLE: Synthesis of 8,9-dialkoxybenzodiazepines and 7,8-dialkoxyisoquinolines
AUTHOR(S): Pongo, Laszlo; Agai, Bela; Faigl, Ferenc; Reiter, Jozsef; Simig, Gyula
CORPORATE SOURCE: Chemical Research Division, Egis Pharmaceuticals Ltd., Budapest, H-1475, Hung.
SOURCE: Journal of Heterocyclic Chemistry (2006), 43(6), 1539-1547
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

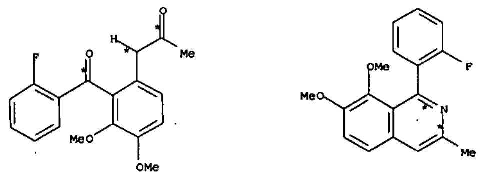


I

AB O-Aroylarylacetone type 1,5-diketone derivs. were synthesized from arylacetones protected as 1,3-dioxolanes through directed ortho lithiation followed by acylation with aroyl chlorides. 8,9-Dialkoxy-2,3-benzodiazepines, e.g., I, were obtained by cyclization of diketones with hydrazine. The reaction of diketones with ammonia gave 7,8-dialkoxyisoquinolines. Reaction of ketals with hydrazine hydrochloride and hydroxylamine hydrochloride afforded N-amino-7,8-dialkoxyisoquinolinium chlorides and 7,8-dialkoxyisoquinolinium oxides, resp.

RX(47) OF 161 ...AI ===> BV

L2 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



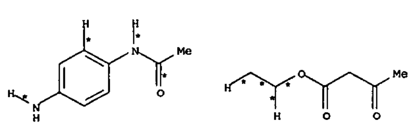
AI

(47) → BV
YIELD 58%

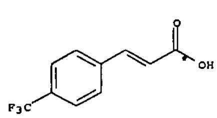
RX(47) RCT AI 924280-03-5
RGT BW 7664-41-7 NH3
PRO BV 924280-37-5
SOL 7732-18-5 Water, 67-56-1 MeOH
CON 1 hour, reflux
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 145:483225 CASREACT
TITLE: 4-Aminoquinoline melanin-concentrating hormone 1-receptor (MCH1R) antagonists
AUTHOR(S): Jiang, Jinlong; Lin, Peter; Hoang, Myle; Chang, Lehua; Tan, Carina; Feighner, Scott; Palyha, Oksana C.; Hreniuk, Donna L.; Pan, Jie; Sailer, Andreas W.; Morin, Nancy R.; MacNeil, Douglas J.; Howard, Andrew D.; Van der Ploeg, Lex H. T.; Goulet, Mark T.; DeVita, Robert J.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065-0900, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(20), 5275-5279
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Structure-activity relationships of a 4-aminoquinoline MCH1R antagonist lead series were explored by synthesis of analogs with modifications at the 2-, 4-, and 6-positions of the original HTS hit. Improvements to the original screening lead included lipophilic groups at the 2-position and biphenyl, cyclohexyl Ph, and hydrocinnamyl carboxamides at the 6-position.
Modifications of the 4-amino group were not well tolerated.

RX(31) OF 51 A + BQ + Y ===> BR



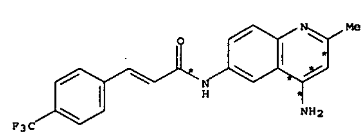
A BQ



Y

(31) →

L2 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BR

RX(31) RCT A 122-80-5, BQ 141-97-9

STAGE(1)
CAT 12408-02-5 H+
SOL 64-17-5 EtOH
CON reflux

STAGE(2)
SOL 101-84-8 PhOPh
CON heated

STAGE(3)
RGT E 77-78-1 Me2SO4
SOL 108-88-3 PhMe
CON reflux

STAGE(4)
RGT F 631-61-8 NH4OAc
CON 150 deg C

STAGE(5)
RCT Y 16642-92-5

PRO BR 137872-88-9
NTE reactant assumed
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

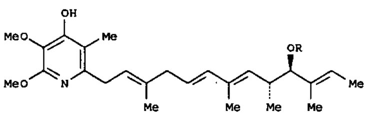
ACCESSION NUMBER: 145:438435 CASREACT

TITLE: Total Synthesis of Piericidin A1 and B1 and Key Analogues

AUTHOR(S): Schnermann, Martin J.; Romero, F. Anthony; Hwang, Inkyu; Nakamaru-Ogiso, Eiko; Yagi, Takao; Boger, Dale L.
CORPORATE SOURCE: Departments of Chemistry and Molecular and Experimental Medicine and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SOURCE: Journal of the American Chemical Society (2006), 128(36), 11799-11807
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



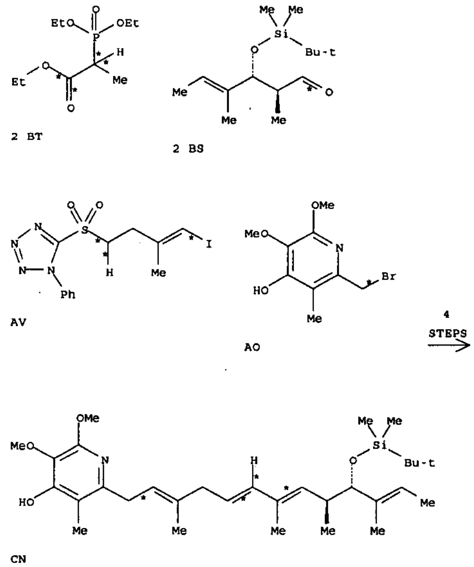
I

AB Piericidin A1 and B1 I (R = H, Me) and analogs with modified side chains and pyridine cores (and the enantiomer of piericidin A1) are prepared enantioselectively; the effect of structural changes on the inhibition of mitochondrial complex I (ubiquinone reductase) and on their cytotoxicities in mouse leukemia cell line L1210 are determined The key step in the synthesis of I (R = H, Me) and their analogs is the inverse electron-demand hetero-Diels-Alder reactions of α-(sulfonylimino)-β,γ-unsatd. esters with tetramethoxyethene followed by elimination of the sulfonyl group, a proton, and two methoxy groups in the presence of boron trifluoride etherate to yield functionalized dimethoxypyridinecarboxylates which are oxidized to the piericidin core by a lithiation/boronation/oxidation sequence. The side chains of I (R = H, Me) and their nonracemic analogs are prepared by use of stereoselective aldol addns. of nonracemic propanoyloxazolidinones and by stereoselective Julia couplings of allylic phenyltetrazolyl sulfones with nonracemic aldehydes. The fully elaborated side chains are prepared as alkenylstannanes; Stille coupling reactions with bromomethylpyridines in the presence of palladium catalysts generates protected piericidins and their analogs which are converted to the desired products. While simplified analogs of I inhibit mitochondrial complex I with similar affinities, the cytotoxicities of analogs of I in mouse leukemia cell line L1210 vary with structural

L2 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

changes in the side chain and in the pyridine core,. The crystal structures of a tetrahydropyridinecarboxylate and of an α-(triisopropylsilyl)pyridinemethanol, intermediates in the prepn. of I (R = H, Me), are detd. by X-ray crystallog.

RX(185) OF 553 COMPOSED OF RX(22), RX(24), RX(27), RX(30)
RX(185) 2 BT + 2 BS + AV + AO ===> CN



RX(22) RCT BT 3699-66-9

STAGE(1)

L2 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RGT BW 7646-69-7 NaH
SOL 109-99-9 THF
CON 10 minutes, 0 deg C

STAGE(2)
RCT BS 134833-55-9
CON SUBSTAGE(1) 0 deg C -> 25 deg C
SUBSTAGE(2) 18 hours, 25 deg C

STAGE(3)
RGT X 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C -> 0 deg C
SUBSTAGE(2) 1 hour, 0 deg C

STAGE(4)
RGT C 67-56-1 MeOH, BX 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON 0 deg C -> 25 deg C

PRO BU 134833-58-2, BV 871316-31-3
NTE stereoselective

RX(24)

STAGE(1)
RGT A 79-37-8 (COCl)2, CA 67-68-5 DMSO
SOL 75-09-2 CH2Cl2
CON 10 minutes, -78 deg C

STAGE(2)
RCT BU 134833-58-2
SOL 75-09-2 CH2Cl2
CON 10 minutes, -78 deg C

STAGE(3)
RGT E 121-44-8 Et3N
CON SUBSTAGE(1) 5 minutes, -78 deg C
SUBSTAGE(2) -78 deg C -> 25 deg C

PRO BZ 871316-23-3
NTE Swern oxidn.

RX(27) RCT AV 871316-22-2

STAGE(1)
RGT CD 40949-94-8 K [N(SiMe3)2]
SOL 110-71-4 (CH2OMe)2
CON 20 minutes, -60 deg C

STAGE(2)
RCT BZ 871316-23-3
SOL 110-71-4 (CH2OMe)2
CON SUBSTAGE(1) 7 hours, -60 deg C
SUBSTAGE(2) -60 deg C -> 25 deg C

PRO CF 912877-26-0
NTE stereoselective, modified Julia coupling

L2 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
RX(30) RCT CF 912877-26-0

STAGE(1)
RGT AD 109-72-8 BuLi
SOL 60-29-7 Et2O
CON 20 minutes, -78 deg C

STAGE(2)
RGT CG 1461-22-9 Bu3SnCl
CON SUBSTAGE(1) 20 minutes, -78 deg C
SUBSTAGE(2) -78 deg C -> 25 deg C

STAGE(3)
RCT AO 871316-20-0
RGT CJ 7447-41-8 LiCl
CAT 13716-12-6 t-Bu3P, 51364-51-3 Ph2-pentadienone Pd
SOL 123-91-1 Dioxane
CON SUBSTAGE(1) room temperature -> 70 deg C
SUBSTAGE(2) 18 hours, 70 deg C

PRO CN 912877-27-1
NTE stereoselective 3rd stage, Stille coupling 3rd stage

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:249128 CASREACT

TITLE: Antibacterial activity of pyrrolopyridine-substituted oxazolidinones: synthesis and in vitro SAR of various C-5 acetamide replacements

AUTHOR(S): Paget, Steven D.; Boggs, Christine M.; Foleno, Barbara D.; Goldschmidt, Raul M.; Hlasta, Dennis J.; Weidner-Wells, Michele A.; Werblood, Harvey M.; Bush, Karen; Macielag, Mark J.

CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research and Development, L.L.C., Raritan, NJ, 08869, USA

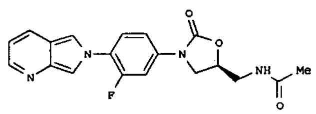
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(17), 4537-4542
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

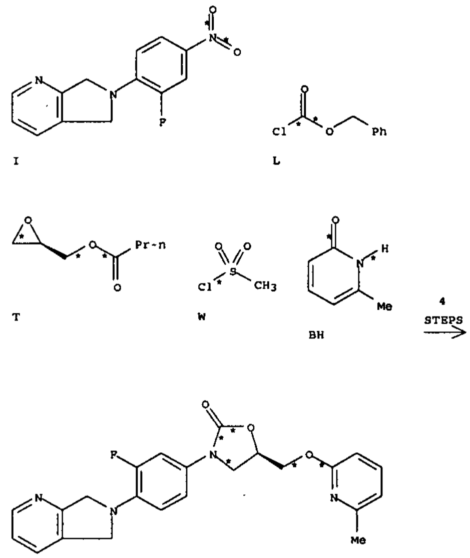


I

AB A series of pyrrolopyridine-substituted oxazolidinones containing various C-5 acetamide isosteres, e.g. I, was synthesized and the structure-antibacterial activity relationships were determined against a representative panel of susceptible and resistant Gram-pos. bacteria.

RX(66) OF 167 COMPOSED OF RX(4), RX(5), RX(6), RX(21)
RX(66) I + L + T + W + BH ===> BI

L2 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



BI
YIELD 93%

RX(4) RCT I 344460-40-8

STAGE(1)
RGT N 540-69-2 Ammonium formate
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH, 109-99-9 THF

STAGE(2)
RCT L 501-53-1

L2 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RGT O 144-55-8 NaHCO3
SOL 7732-18-5 Water, 67-64-1 Me2CO

PRO M 344460-43-1

RX(5) RCT M 344460-43-1

STAGE(1)
RGT V 109-72-8 BuLi
SOL 109-99-9 THF
CON -78 deg C

STAGE(2)
RCT T 60456-26-0
CON -78 deg C -> room temperature

PRO U 344459-52-5

RX(6) RCT U 344459-52-5, W 124-63-0
RGT Y 121-44-8 Et3N
PRO X 344460-45-3
SOL 68-12-2 DMF
NTE key intermediate

RX(21) RCT X 344460-45-3, BH 3279-76-3
RGT BG 7646-69-7 NaH
PRO BI 906480-77-1
SOL 68-12-2 DMF

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:8155 CASREACT

TITLE: Preparation of 1,7-naphthyridines as selective PDE4 inhibitors for treating and/or preventing an inflammatory and/or allergic diseases

INVENTOR(S): Eldred, Colin David; Robinson, John Edward; Steel, Alison Judith

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006053784	A2	20060526	WO 2005-EP12462	20051117
WO 2006053784	A3	20060706		

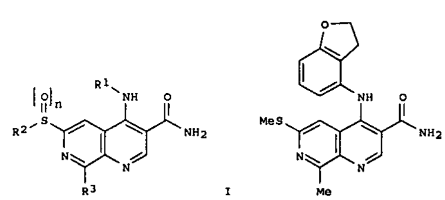
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2004-25572 20041119

OTHER SOURCE(S): MARPAT 145:8155

GI

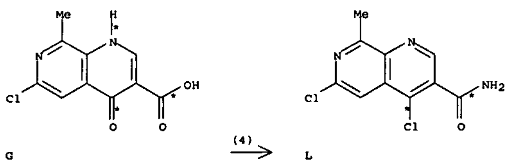


I II

AB The title compds. I [R1 = Ph which may be unsubstituted or substituted by one or two substituents selected from F, Cl, alkoxy, CN; Ph fused to a 5-membered saturated ring containing one O atom; pyridinyl which may be unsubstituted or substituted by one or two substituents selected from F or Cl; or C-linked pyrazolyl which may be unsubstituted or substituted by

L2 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
alkyl; R2 = alkyl; R3 = alkyl; and n = 0-2], were prepd. E.g., a multi-step synthesis of II, starting from 6-chloro-2-methyl-3-pyridinamine and di-Et [(ethoxy)methylidene]propanedioate, was given. The ability of compds. I to inhibit PDE3, PDE4B, PDE4D, PDE5 and PDE6 was detd. (data were given for exemplified compds. I). For example, II showed pIC50 of 9.5 in PDE4B and PDE4D assays. Pharmaceutical compn. comprising the compd. I was disclosed.

RX(4) OF 35 ...G ===> L...



RX(4) RCT G 888011-95-8

STAGE(1)
RGT M 10025-87-3 POCl3
SOL 10025-87-3 POCl3
CON overnight, 50 deg C

STAGE(2)
RGT N 7664-41-7 NH3
SOL 67-56-1 MeOH, 109-99-9 THF
CON SUBSTAGE(1) 10 minutes, -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C
SUBSTAGE(3) overnight, -78 deg C -> room temperature

PRO L 888011-96-9

=> d ibib abs kwic 1-3

L12 ANSWER 1 OF 3 CA COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 142:113907 CA
TITLE: Catalytic process for the production of pyridine and picolines from ammonia and carbonyl compounds
INVENTOR(S): Kumar, Rajiv; Joshi, Praphulla Narahar; Chapekar, Gopal Moreshwar; Niphadkar, Prashant Suresh; Agarwal, Ashutosh; Verma, Pradeep Kumar; Singh, Kumar Samir
PATENT ASSIGNEE(S): Council of Scientific and Industrial Research, India; Jubilant Organosys Ltd.
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005000816	A1	20050106	WO 2003-IN465		20031231
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
US 2005131235	A1	20050616	US 2003-731440		20031210
AU 2003300721	A1	20050113	AU 2003-300721		20031231
EP 1648869	A1	20060426	EP 2003-817293		20031231
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
PRIORITY APPLN. INFO.:			IN 2003-DE853	A	20030627
			WO 2003-IN465	W	20031231

OTHER SOURCE(S): CASREACT 142:113907
AB A process for the preparation of pyridine and/or picolines (e.g., a mixture of α- picoline and γ- picoline) is described which comprises contacting a mixture of a carbonyl compound (e.g., acetaldehyde) with ammonia in the presence of a surface-passivated titanium silicate catalyst in gas phase at 300-500°/1-10 bar, a gas space velocity of 300-3000 h-1, condensing and separating the products by conventional methods and if desired, further purifying the product using conventional methods.
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
TI Catalytic process for the production of pyridine and picolines from ammonia and carbonyl compounds

L12 ANSWER 1 OF 3 CA COPYRIGHT 2007 ACS on STN (Continued)
AB A process for the preparation of pyridine and/or picolines (e.g., a mixture of α- picoline and γ- picoline) is described which comprises contacting a mixture of a carbonyl compound (e.g., acetaldehyde) with ammonia in the presence of a surface-passivated titanium silicate catalyst in gas phase at 300-500°/1-10 bar, a gas space velocity of 300-3000 h-1, condensing and separating the products by conventional methods and if desired, further purifying the product using conventional methods.
ST pyridine picoline catalytic prepn; catalyst prepn pyridine picoline
IT Aldehydes, reactions
Carbonyl compounds (organic), reactions
Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic process for the production of pyridine and picolines from ammonia and carbonyl compds.)
IT Heterocyclic compounds
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(nitrogen, pyridine and picolines; catalytic process for the production of pyridine and picolines from ammonia and carbonyl compds.)
IT Catalysts
(surface-passivated titanium silicate for the production of pyridine and picolines from ammonia and carbonyl compds.)
IT 1344-28-1, Alumina, uses 7631-86-9, Silica, uses
RL: CAT (Catalyst use); USES (Uses)
(binder; catalyst in a process for the production of pyridine and picolines from ammonia and carbonyl compds.)
IT 7439-92-1, Lead, uses 7440-02-0, Nickel, uses 7440-28-0, Thallium, uses
RL: CAT (Catalyst use); USES (Uses)
(catalyst in a process for the production of pyridine and picolines from ammonia and carbonyl compds.)
IT 78-10-4DP, Tetra(ethoxy)silane, surface-passivated titanium silicate compns. 681-84-5DP, Tetra(methoxy)silane, surface-passivated titanium silicate compns. 1992-48-9DP, Tetra(isopropoxy)silane, surface-passivated titanium silicate compns. 4766-57-8DP, Tetra(butoxy)silane, surface-passivated titanium silicate compns. 5593-70-4DP, Titanium tetrabutoxide, surface-passivated titanium silicate compns. 10026-04-7DP, Tetrachlorosilane, surface-passivated titanium silicate compns. 11099-06-2DP, Ethyl silicate, surface-passivated titanium silicate compns. 42613-21-8DP, Titanium silicate, surface-passivated compns.
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalyst in a process for the production of pyridine and picolines from

L12 ANSWER 1 OF 3 CA COPYRIGHT 2007 ACS on STN (Continued)
ammonia and carbonyl compds.)
IT 108-89-4P, γ- Picoline 109-06-8P, α- Picoline 110-86-1P, Pyridine, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(catalytic process for the production of pyridine and picolines from ammonia and carbonyl compds.)
IT 50-00-0, Formaldehyde, reactions 67-64-1, Acetone, reactions 75-07-0, Acetaldehyde, reactions 123-38-6, Propionaldehyde, reactions 7664-41-7, Ammonia, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic process for the production of pyridine and picolines from ammonia and carbonyl compds.)

L12 ANSWER 2 OF 3 CA COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 116:135528 CA
TITLE: Performance-oriented packaging standards; changes to classification, hazard communication, packaging and handling requirements based on UN standards and agency initiative
CORPORATE SOURCE: United States Dept. of Transportation, Washington, DC, 20590-0001, USA
SOURCE: Federal Register (1990), 55(246), 52402-729, 21 Dec 1990
CODEN: FEREAC; ISSN: 0097-6326
DOCUMENT TYPE: Journal
LANGUAGE: English
SYSTEM LIMIT EXCEEDED DURING KWIC/STRING SEARCH
AB The hazardous materials regulations under the Federal Hazardous Materials Transportation Act are revised based on the United Nations recommendations on the transport of dangerous goods. The regulations cover the classification of materials, packaging requirements, and package marking, labeling, and shipping documentation, as well as transportation modes and handling, and incident reporting. Performance-oriented stds. are adopted for packaging for bulk and nonbulk transportation, and SI units of measurement generally replace US customary units. Hazardous material descriptions and proper shipping names are tabulated together with hazard class, identification nos., packing group, label required, special provisions, packaging authorizations, quantity limitations, and vessel stowage requirements.
IT 50-00-0, Formaldehyde, miscellaneous 54-11-5, Nicotine 54-11-5D, Nicotine, compds. 55-63-0, Nitroglycerin 55-68-5, Phenylmercuric nitrate 56-18-8, 3,3'-Iminodipropylamine 56-23-5, miscellaneous 56-38-2, Parathion 57-06-7, Allyl isothiocyanate 57-14-7 57-24-9D, Strychnine, salts 60-00-4, EDTA, miscellaneous 60-24-2 60-29-7, Diethyl ether, miscellaneous 60-34-4, Methylhydrazine 60-57-1, Dieldrin 62-38-4, Phenylmercuric acetate 62-53-3, Aniline, miscellaneous 62-74-8, Sodium fluoroacetate 64-17-5, Ethanol, miscellaneous 64-18-6, Formic acid, miscellaneous 64-18-6D, Formic acid, chloro derivs. 64-19-7, Acetic acid, miscellaneous 64-67-5, Diethyl sulfate 66-25-1, Hexaldehyde 67-56-1, Methanol, miscellaneous 67-63-0, Isopropanol, miscellaneous 67-64-1, Acetone, miscellaneous 67-66-3, Chloroform, miscellaneous 68-11-1, Thioglycolic acid, miscellaneous 68-12-2, N,N-Dimethylformamide, miscellaneous 70-11-1, Phenacyl bromide 70-30-4, Hexachlorophene 71-23-8, n-Propanol, miscellaneous 71-41-0, 1-Pentanol, miscellaneous 71-43-2, Benzene, miscellaneous 71-55-6, 1,1,1-Trichloroethane 74-82-8, Methane, miscellaneous 74-83-9, miscellaneous 74-84-0, Ethane, miscellaneous 74-85-1, Ethylene, miscellaneous 74-86-2, Acetylene, miscellaneous 74-87-3, Methyl chloride, miscellaneous 74-88-4, Methyl iodide, miscellaneous 74-89-5, Methylamine, miscellaneous 74-90-8, Hydrogen cyanide, miscellaneous 74-93-1, Methyl mercaptan, miscellaneous 74-95-3, Dibromomethane 74-96-4, Ethyl bromide 74-97-5, Bromochloromethane 74-98-6, Propane, miscellaneous 75-00-3, Ethyl chloride 75-01-4, miscellaneous 75-02-5, Vinyl fluoride 75-04-7, Ethylamine, miscellaneous 75-05-8, Methyl cyanide, miscellaneous 75-07-0, Acetaldehyde, miscellaneous 75-08-1, Ethyl mercaptan 75-09-2, Dichloromethane, miscellaneous 75-15-0, Carbon disulfide, miscellaneous 75-16-1, Methyl magnesium bromide 75-18-3, Dimethyl sulfide 75-19-4, Cyclopropane 75-20-7, Calcium carbide 75-21-8, Ethylene oxide,

miscellaneous 75-21-8 75-25-2, Bromoform 75-26-3, 2-Bromopropane 75-28-5, Isobutane 75-28-5D, Isobutane, mixts. 75-29-6, 2-Chloropropane 75-31-0, Isopropylamine, miscellaneous 75-33-2, Isopropyl mercaptan 75-34-3, 1,1-Dichloroethane 75-35-4, miscellaneous
75-36-5, Acetyl chloride 75-38-7, 1,1-Difluoroethylene 75-39-8, Acetaldehyde ammonia 75-43-4, Dichloromonofluoromethane 75-44-5, Phosgene 75-45-6, Chlorodifluoromethane 75-46-7, Trifluoromethane 75-50-3, Trimethylamine, miscellaneous 75-52-5, Nitromethane, miscellaneous 75-54-7, Methyldichlorosilane 75-55-8, Propylenimine 75-56-9, Propylene oxide, miscellaneous 75-59-2, Tetramethylammonium hydroxide 75-60-5, Cacodylic acid 75-61-6, Dibromodifluoromethane 75-63-8 75-71-8, Dichlorodifluoromethane 75-72-9, Chlorotrifluoromethane 75-73-0, Tetrafluoromethane 75-76-3, Tetramethylsilane 75-77-4, Trimethylchlorosilane, miscellaneous 75-78-5, Dimethyldichlorosilane 75-79-6, Methyltrichlorosilane
75-83-2
75-86-5, Acetone cyanohydrin 75-87-6, Chloral 75-91-2, tert-Butyl hydroperoxide 75-94-5, Vinyltrichlorosilane 76-01-7,
Pentachloroethane
76-02-8, Trichloroacetyl chloride 76-03-9, properties 76-05-1, Trifluoroacetic acid, miscellaneous 76-06-2, Chloropicrin 76-06-2D, Chloropicrin, mixts. 76-15-3 76-16-4, Hexafluoroethane 76-19-7, Octafluoropropane 76-22-2, Camphor 77-47-4, Hexachlorocyclopentadiene 77-73-6 77-78-1, Dimethyl sulfate 78-00-2, Tetraethyl lead 78-10-4, Tetraethyl silicate 78-62-6, Dimethyldiethoxysilane 78-67-1, Azodiisobutyronitrile 78-76-2, 2-Bromobutane 78-78-4, Isopentane 78-79-5, Isoprene, miscellaneous 78-81-9, Isobutylamine 78-82-0, Isobutyronitrile 78-83-1, Isobutanol, miscellaneous 78-84-2, Isobutyraldehyde 78-85-3, Methacrylaldehyde 78-87-5, Propylene dichloride 78-89-7, Propylene chlorohydrin 78-90-0, 1,2-Propylenediamine 78-93-3, 2-Butanone, miscellaneous 78-94-4, Methyl vinyl ketone, miscellaneous 78-95-5, Monochloroacetone
79-01-6,
Trichloroethylene, miscellaneous 79-03-8, Propionyl chloride 79-04-9, Chloroacetyl chloride 79-06-1, Acrylamide, miscellaneous 79-08-3, Bromoacetic acid 79-09-4, Propionic acid, miscellaneous 79-10-7, 2-Propenoic acid, miscellaneous 79-11-8, Chloroacetic acid, miscellaneous 79-20-9, Methyl acetate 79-21-0, Peroxyacetic acid 79-22-1 79-24-3, Nitroethane 79-29-8, 2,3-Dimethylbutane 79-30-1, Isobutyryl chloride 79-31-2, Isobutyric acid 79-36-7, Dichloroacetyl chloride 79-38-9 79-41-4, miscellaneous 79-42-5 79-43-6, Dichloroacetic acid, miscellaneous 79-44-7, Dimethylcarbamoyl chloride 80-10-4, Diphenyldichlorosilane 80-15-9, Cumene hydroperoxide
80-17-1,
Benzene sulfohydrazide 80-47-7, p-Menthane hydroperoxide 80-51-3, Diphenyloxide-4,4'-disulfohydrazide 80-56-8, α-Pinene 80-62-6 81-15-2 82-71-3 85-44-9, 1,3-Isobenzofurandione 86-50-0, Azinphos methyl 87-68-3, Hexachlorobutadiene 87-90-1 88-17-5, 2-Trifluoromethylaniline 88-72-2, o-Nitrotoluene 88-73-3, o-Chloronitrobenzene 88-74-4, o-Nitroaniline 88-75-5, o-Nitrophenol 88-89-1 89-58-7, p-Nitroxylene 91-17-8, Decahydronaphthalene 91-20-3, Naphthalene, miscellaneous 91-20-3D, Naphthalene, diozonide derivs. 91-22-5, Quinoline, miscellaneous 91-59-8, β-Naphthylamine 91-66-7, N,N-Diethylaniline 92-52-4D, Biphenyl,

chloro derivs. 92-52-4D, Biphenyl, halo derivs. 92-59-1, N-Ethyl-N-benzylaniline 92-87-5, Benzidine 93-58-3, Methyl benzoate 94-17-7, p-Chlorobenzoyl peroxide 94-36-0, Benzoyl peroxide, miscellaneous 95-48-7, miscellaneous 95-50-1, o-Dichlorobenzene 95-54-5, o-Phenylenediamine, miscellaneous 95-55-6, o-Aminophenol 95-80-7 95-85-2, 2-Amino-4-chlorophenol 96-12-8, Dibromochloropropane 96-22-0, Diethyl ketone 96-23-1 96-24-2, Glycerol α-monochlorohydrin 96-32-2, Methyl bromoacetate 96-33-3 96-34-4, Methyl chloroacetate 96-37-7, Methyl cyclopentane 96-41-3, Cyclopentanol 97-62-1, Ethyl isobutyrate 97-63-2 97-64-3, Ethyl lactate 97-72-3, Isobutyric anhydride 97-85-8, Isobutyl isobutyrate 97-86-9 97-88-1 97-95-0 97-96-1, 2-Ethylbutyraldehyde 98-00-0, Furfuryl alcohol 98-01-1, Furfural, miscellaneous 98-07-7, Benzotrichloride 98-08-8, Benzotrifluoride 98-09-9, Benzene sulfonyl chloride 98-12-4, Cyclohexyltrichlorosilane 98-13-5, Phenyltrichlorosilane 98-16-8, 3-Trifluoromethylaniline 98-82-8, Isopropylbenzene 98-83-9, miscellaneous 98-85-1, α-Methylbenzyl alcohol 98-87-3, Benzylidene chloride 98-88-4, Benzoyl chloride 98-94-2 98-95-3, Nitrobenzene, miscellaneous 99-08-1, m-Nitrotoluene 99-09-2, m-Nitroaniline 99-35-4, Trinitrobenzene 99-99-0, p-Nitrotoluene 100-00-5 100-01-6, p-Nitroaniline, miscellaneous 100-02-7, p-Nitrophenol, miscellaneous 100-17-4 100-34-5, Benzene diazonium chloride
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(packaging and transport of, stds. for)

IT 138-86-3, Dipentene 138-89-6 139-02-6, Sodium phenolate 140-29-4, Phenylacetonitrile 140-31-8, 1-Piperazineethanamine 140-80-7 140-88-5 141-32-2 141-43-5, Ethanolamine, miscellaneous 141-57-1, Propyltrichlorosilane 141-59-3, tert-Octylmercaptan 141-75-3, Butyryl chloride 141-78-6, Ethyl acetate, miscellaneous 141-79-7, Mesityl oxide 142-04-1, Aniline hydrochloride 142-29-0, Cyclopentene 142-62-1, Hexanoic acid, miscellaneous 142-82-5, Heptane, miscellaneous 142-84-7, Dipropylamine 142-96-1, Dibutyl ether 143-33-9, Sodium cyanide 144-49-0, Fluoroacetic acid 144-62-7D, Ethanedioic acid,
salts
146-84-9, Silver picrate 149-74-6, Methylphenyldichlorosilane 151-50-8, Potassium cyanide 151-56-4, Ethylenimine, miscellaneous 156-62-7, Calcium cyanamide 260-94-6, Acridine 283-66-9,
Hexamethylene
triperoxide diamine 287-23-0, Cyclobutane 287-92-3, Cyclopentane 291-64-5, Cycloheptane 298-00-0, Methyl parathion 298-07-7
302-01-2,
Hydrazine, miscellaneous 309-00-2, Aldrin 352-93-2, Diethyl sulfide 353-36-6, Ethyl fluoride 353-42-4, Boron trifluoride dimethyl etherate 353-50-4, Carbonyl fluoride 353-59-3 354-32-5, Trifluoroacetylchloride 357-57-3, Brucine 360-89-4, Octafluorobut-2-ene 428-59-1, Hexafluoropropylene oxide 431-03-8, Butanedione 460-19-5, Cyanogen 462-06-6, Fluorobenzene 462-08-8, m-Aminopyridine 462-95-3, Diethoxymethane 463-04-7, Amyl nitrite 463-49-0, Propadiene 463-58-1, Carbonyl sulfide 463-71-8, Thiophosgene 463-82-1, 2,2-Dimethylpropane 479-45-8 501-53-1,
Benzyl
chloroformate 502-98-7D, salts 503-74-2, Isopentanoic acid
504-24-5,

4-Pyridinamine 504-29-0, 2-Pyridinamine 506-64-9, Silver cyanide (Ag(CN)) 506-68-3, Cyanogen bromide 506-77-4, Cyanogen chloride 506-85-4, Fulminic acid 506-93-4, Guanidine nitrate 506-96-7, Acetyl bromide 507-02-8, Acetyl iodide 507-09-5, Thioacetic acid, miscellaneous 507-70-0, Borneol 509-14-8, Tetranitromethane 512-85-6, Ascaridole 513-35-9, 2-Methyl-2-butene 513-38-2 513-42-8, Methallyl alcohol 513-48-4, 2-Iodobutane 513-86-0, Acetyl methyl carbinol 517-25-9, Trinitromethane 517-92-0, 1,8-Dihydroxy-2,4,5,7-tetranitroanthraquinone 519-44-8D, 2,4-Dinitroresorcinol, heavy metal salts 532-27-4, Chloracetophenone 533-51-7, Silver oxalate
534-07-6,
1,3-Dichloroacetone 534-15-6, 1,1-Dimethoxyethane 534-22-5, 2-Methylfuran 535-13-7, Ethyl-2-chloropropionate 540-18-1, Amyl butyrate 540-42-1, Isobutyl propionate 540-54-5, Propyl chloride 540-67-0, Ethyl methyl ether 540-73-8 540-82-9, Ethylsulfuric acid 540-84-1, Isooctane 541-41-3, Ethyl chloroformate 542-55-2, Isobutyl formate 542-62-1, Barium cyanide 542-88-1, Dichlorodimethyl ether, symmetrical 543-27-1, Isobutyl chloroformate 543-59-9, Amyl chloride 544-16-1, Butyl nitrite 544-25-2, Cycloheptatriene 544-97-8, Dimethyl zinc 545-55-1, Tris(1-aziridinyl)phosphine oxide 554-12-1, Methyl propionate 554-84-7, m-Nitrophenol 555-54-4, Magnesium diphenyl 556-24-1, Methyl isovalerate 556-56-9, Allyl iodide 556-61-6, Methyl isothiocyanate 556-88-7 556-89-8, Nitrourea 557-17-5, Methyl propyl ether 557-19-7, Nickel cyanide (Ni(CN)2) 557-20-0, Diethylzinc 557-21-1, Zinc cyanide 557-31-3, Allyl ethyl ether 557-40-4, Diallylether 557-98-2, 2-Chloropropene 558-13-4, Carbon tetrabromide 563-45-1, 3-Methyl-1-butene 563-46-2, 2-Methyl-1-butene 563-47-3, Methyl allyl chloride 563-80-4, 3-Methylbutan-2-one 578-54-1, 2-Ethylaniline 578-94-9, Diphenylamine chloroarsine 582-61-6, Benzoyl azide 583-15-3, Mercury benzoate 584-79-2, Allethrin 585-79-5, 1-Bromo-3-nitrobenzene 586-62-9, Terpinolene 587-85-9D, compds. 590-01-2, Butylpropionate 590-36-3, 2-Methylpentan-2-ol 591-27-5, m-Aminophenol 591-87-7, Allyl acetate 591-89-9, Mercuric potassium cyanide 592-01-8, Calcium cyanide 592-05-2, Lead cyanide (Pb(CN)2) 592-34-7, n-Butylchloroformate 592-41-6, 1-Hexene, miscellaneous 592-55-2, 2-Bromoethyl ethyl ether 592-63-2 592-84-7, n-Butylformate 593-53-3, Methyl fluoride 593-60-2, Vinyl bromide 593-89-5, Methyldichloroarsine 594-42-3, Perchloromethylmercaptan 594-72-9, 1,1-Dichloro-1-nitroethane 598-14-1, Ethyldichloroarsine 598-21-0, Bromoacetyl bromide 598-31-2, Bromoacetone 598-57-2, Methyl nitramine 598-57-2D, Methyl nitramine, metal salts 598-58-3, Methyl nitrate 598-73-2, Bromotrifluoroethylene 598-78-7, α-Chloropropionic acid 598-99-2, Methyl trichloroacetate 602-96-0, 1,3,5-Trimethyl-2,4,6-trinitrobenzene 602-99-3, Trinitro-m-cresol 602-99-3D, Methyl picric acid, heavy metal salts 608-50-4, 2,4-Dinitro-1,3,5-trimethylbenzene 610-38-8, 4-Bromo-1,2-dinitrobenzene 616-38-6, Dimethyl carbonate 616-74-0D, 4,6-Dinitroresorcinol, heavy metal salts 617-37-8
617-50-5,
Isopropyl isobutyrate 617-89-0, Furfurylamine 619-97-6, Benzene diazonium nitrate 620-05-3, Benzyl iodide 622-44-6, Phenylcarbylamine chloride 622-45-7, Cyclohexyl acetate 623-42-7, Methyl butyrate 623-87-0, Glycerol-1,3-dinitrate 624-61-3, Dibromoacetylene 624-74-8, Diiodoacetylene 624-83-9, Methyl isocyanate 624-91-9, Methyl nitrite 624-92-0, Dimethyl disulfide 625-76-3, Dinitromethane 626-67-5, 1-Methylpiperidine 627-13-4, n-Propyl nitrate 627-30-5 627-63-4, Fumaryl chloride 628-28-4, Butyl methyl ether 628-32-0, Ethyl propyl ether 628-63-7, Amyl acetate 628-81-9, Ethyl butyl ether 628-86-4, Mercury fulminate 628-92-2, Cycloheptene 628-96-6, Ethylene glycol dinitrate 629-13-0, 1,2-Diazidoethane 629-14-1 629-20-9,

Cyclooctatetraene 630-08-0, Carbon monoxide, miscellaneous 630-72-8, Trinitroacetonitrile 637-78-5, Isopropyl propionate 638-11-9, Isopropyl butyrate 638-29-9, Valeryl chloride 638-49-3, Amyl formate 641-16-7, 2,3,4,6-Tetranitrophenol 644-31-5, Acetyl benzoyl peroxide 644-97-3, Phenyl phosphorus dichloride 645-55-6, N-Nitroaniline 646-06-0, Dioxolane 674-81-7, Nitrosoguanidine 674-82-8, Diketene 676-83-5, Methyl phosphonous dichloride 676-97-1, Methyl phosphonic dichloride 676-98-2, Methyl phosphonothioic dichloride 677-71-4, Hexafluoroacetone hydrate 681-84-5, Methyl orthosilicate 684-16-2, Hexafluoroacetone 693-21-0, Diethylene glycol dinitrate 694-05-3, 1,2,3,6-Tetrahydropyridine 757-58-4, Hexaethyl tetraphosphate 762-12-9, Decanoyl peroxide 762-13-0, Pelargonyl peroxide 762-16-3 765-34-4, Glycidaldehyde 766-09-6, 1-Ethylpiperidine 771-29-9, Tetralin hydroperoxide 776-74-9, Diphenylmethyl bromide 814-78-8, Methyl isopropenyl ketone 822-06-0 831-52-7, Sodium picramate 883-40-9, Diazodiphenylmethane 918-37-6, Hexanitroethane 918-54-7, Trinitroethanol 926-63-6 926-64-7, 2-Dimethylaminoacetonitrile 928-65-4, Hexyltrichlorosilane 929-06-6, 2-(2-Aminoethoxy)ethanol 993-00-0, Methylchlorosilane 993-12-4 993-43-1, Ethyl phosphonothioic dichloride
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IT 1002-16-0, Amyl nitrate 1070-19-5, tert-Butoxycarbonyl azide 1120-21-4, Undecane 1125-27-5 1126-78-9 1187-93-5, Perfluoromethyl vinyl ether 1299-86-1, Aluminum carbide 1300-64-7, Anisoyl chloride 1300-71-6, Xylenol 1300-73-8D, derivs. 1303-28-2, Arsenic pentoxide 1303-33-9, Arsenic sulfide 1303-33-9D, Arsenic sulfide, mixture with chlorates 1304-28-5, Barium oxide, miscellaneous 1304-29-6, Barium peroxide 1305-78-8, Calcium oxide, miscellaneous 1305-79-9, Calcium peroxide 1305-99-3, Calcium phosphide 1309-60-0, Lead dioxide 1310-58-3, Potassium hydroxide, miscellaneous 1310-65-2, Lithium hydroxide 1310-73-2, Sodium hydroxide, miscellaneous 1310-82-3, Rubidium hydroxide 1312-73-8, Potassium sulfide 1313-60-6, Sodium peroxide 1313-82-2, Sodium sulfide, miscellaneous 1314-18-7,
Strontium
peroxide 1314-22-3, Zinc peroxide 1314-24-5, Phosphorus trioxide 1314-34-7, Vanadium trioxide 1314-56-3, Phosphorus pentoxide, miscellaneous 1314-62-1, Vanadium pentoxide, miscellaneous 1314-80-3, Phosphorus sulfide (P2S5) 1314-84-7, Zinc phosphide 1314-85-8, Phosphorus sesquisulfide 1319-77-3, Cresylic acid 1320-37-2, Dichlorotetrafluoroethane 1321-10-4, Chlorocresol 1321-31-9, Phenetidine 1327-53-3, Arsenic trioxide 1330-20-7, Xylene, miscellaneous 1330-45-6, Chlorotrifluoroethane 1330-78-5, Tricresyl phosphate 1331-22-2, Methyl cyclohexanone 1332-12-3, Fulminating gold 1332-37-2, Iron oxide, properties 1333-39-7, Phenolsulfonic acid 1333-41-1, Picoline 1333-74-0, Hydrogen, miscellaneous 1333-82-0, Chromium trioxide 1333-83-1, Sodium hydrogen fluoride 1335-26-8, Magnesium peroxide 1335-31-5, Mercury oxycyanide
1335-85-9,
Dinitro-o-cresol 1336-21-6, Ammonium hydroxide 1337-81-1 1338-23-4, Methyl ethyl ketone peroxide 1341-24-8, Chloroacetophenone 1341-49-7, Ammonium hydrogen fluoride 1344-40-7, Lead phosphite, dibasic 1344-67-8, Copper chloride 1498-40-4, Ethyl phosphonous dichloride 1498-51-7, Ethyl phosphorodichloridate 1569-69-3, Cyclohexyl mercaptan 1609-86-5, tert-Butyl isocyanate 1623-15-0 1623-24-1, Isopropyl acid phosphate 1634-04-4, Methyl-tert-butyl ether 1693-71-6, Triallyl borate 1705-60-8, 2,2-Di(4,4-di-tert-butylperoxycyclohexyl)propane 1712-64-7, Isopropyl nitrate 1719-53-5, Diethyldichlorosilane

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1737-93-5, 3,5-Dichloro-2,4,6-trifluoropyridine 1789-58-8, Ethyldichlorosilane 1795-48-8, Isopropyl isocyanate 1838-59-1, Allyl formate 1873-29-6, Isobutyl isocyanate 1885-14-9, Phenylchloroformate 1947-27-9, Arsenic trichloride 2050-92-2, Di-n-amylamine 2094-98-6, 1,1'-Azodi(hexahydrobenzonitrile) 2144-45-8, Dibenzyl peroxydicarbonate 2155-71-7 2167-23-9, 2,2-Di(tert-butylperoxy)butane 2217-06-3, Dipicryl sulfide 2243-94-9, 1,3,5-Trinitronaphthalene 2244-21-5, Potassium dichloroisocyanurate 2294-47-5, p-Diazidobenzene 2312-76-7 2338-12-7, 5-Nitrobenzotriazole 2487-90-3, Trimethoxysilane
2508-19-2,
Trinitrobenzenesulfonic acid 2524-03-0, Dimethyl chlorothiophosphate 2524-04-1, Diethylthiophosphoryl chloride 2549-51-1, Vinyl
chloroacetate
2551-62-4, Sulfur hexafluoride 2567-83-1, Tetraethylammonium
perchlorate
2657-00-3, Sodium 2-diazo-1-naphthol-5-sulfonate 2691-41-0, Cyclotetramethylenetetranitramine 2696-92-6, Nitrosyl chloride 2699-79-8, Sulfuryl fluoride 2782-57-2, Dichloroisocyanuric acid 2782-57-2D, Dichloroisocyanuric acid, salts 2820-51-1, Nicotine hydrochloride 2825-15-2 2855-13-2, Isophoronediamine 2867-47-2, Dimethylaminoethyl methacrylate 2893-78-9, Sodium dichloroisocyanurate 2937-50-0, Allyl chloroformate 2941-64-2, Ethyl chlorothioformate 2980-64-5 3025-88-5, 2,5-Dimethyl-2,5-dihydroperoxy hexane 3031-74-1, Ethyl hydroperoxide 3032-55-1 3054-95-3, 3,3-Diethoxypropene 3087-37-4, Tetrapropylorthotitanate 3129-90-6, Isothiocyanic acid 3129-91-7, Dicyclohexylammonium nitrite 3132-64-7, Epibromohydrin 3165-93-3, 4-Chloro-o-toluidine hydrochloride 3173-53-3, Cyclohexyl isocyanate 3179-56-4, Acetyl cyclohexanesulfonyl peroxide 3188-13-4, Chloromethyl ethyl ether 3248-28-0, Dipropionyl peroxide 3268-49-3 3275-73-8, Nicotine tartrate 3282-30-2, Trimethylacetyl chloride 3497-00-5, Phenyl phosphorus thiodichloride 3689-24-5 3724-65-0, Crotonic acid 3811-04-9, Potassium chlorate 3926-62-3, Sodium chloroacetate 3982-91-0, Thiophosphoryl chloride 4016-11-9, 1,2-Epoxy-3-ethoxypropane 4098-71-9 4109-96-0, Dichlorosilane 4170-30-3, Crotonaldehyde 4300-97-4 4316-42-1, N-n-Butylimidazole 4419-11-8, 2,2'-Azodi(2,4-dimethylvaleronitrile) 4421-50-5 4435-53-4, Butoxyl 4452-58-8, Sodium percarbonate 4472-06-4, Carbonazidodithioic acid 4484-72-4, Dodecyltrichlorosilane 4528-34-1 4547-70-0 4591-46-2 4682-03-5, Diazodinitrophenol 4795-29-3, Tetrahydrofurfurylamine 4904-61-4, 1,5,9-Cyclododecatriene 5283-66-9, Octyltrichlorosilane 5283-67-0, Nonyltrichlorosilane 5329-14-6, Sulfamic acid 5419-55-6, Triisopropyl borate 5610-59-3, Silver fulminate 5637-83-2, Cyanuric triazide 5653-21-4 5894-60-0, Hexadecyltrichlorosilane 5970-32-1, Mercury salicylate 6023-29-6 6275-02-1 6423-43-4 6427-21-0, Methoxymethyl isocyanate 6484-52-2, Nitric acid ammonium salt, properties 6484-52-2D, Ammonium nitrate, mixts. with fuel oils 6505-86-8, Nicotine sulfate 6659-60-5, 1,2,4-Butanetriol trinitrate 6842-15-5, Propylene tetramer 6867-30-7, Lithium acetylide ethylenediamine complex 7304-92-9 7332-16-3, Inositol hexanitrate 7429-90-5, Aluminum, miscellaneous 7429-90-5D, Aluminum, alkyl derivs. 7439-90-9, Krypton, miscellaneous 7439-92-1D, Lead, compds. 7439-93-2, Lithium, miscellaneous 7439-93-2D, Lithium, alkyl derivs. 7439-95-4, Magnesium, miscellaneous 7439-95-4D, Magnesium, alkyl derivs. 7439-97-6, Mercury, miscellaneous
7439-97-6D,

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Mercury, compds. 7440-01-9, Neon, miscellaneous 7440-09-7, Potassium, miscellaneous 7440-17-7, Rubidium, miscellaneous 7440-21-3, Silicon, miscellaneous 7440-23-5, Sodium, miscellaneous 7440-28-0D, Thallium, compds. 7440-29-1, Thorium, miscellaneous 7440-31-5D, Tin, org. compds. 7440-32-6, Titanium, properties 7440-36-0, Antimony, miscellaneous 7440-36-0D, Antimony, inorg. and org. compds.
7440-37-1,
Argon, miscellaneous 7440-38-2, Arsenic, miscellaneous 7440-39-3, Barium, miscellaneous 7440-39-3D, Barium, alloys 7440-39-3D, Barium, compds. 7440-41-7, Beryllium, miscellaneous 7440-41-7D, Beryllium, compds. 7440-43-9D, Cadmium, compds. 7440-44-0, Carbon, miscellaneous 7440-45-1, Cerium, miscellaneous 7440-46-2, Cesium, miscellaneous 7440-55-3, Gallium, miscellaneous 7440-58-6, Hafnium, miscellaneous 7440-59-7, Helium, miscellaneous 7440-61-1, Uranium, miscellaneous 7440-63-3, Xenon, miscellaneous 7440-66-6, Zinc, miscellaneous 7440-67-7, Zirconium, miscellaneous 7440-70-2, Calcium, miscellaneous 7440-70-2D, Calcium, alloys 7446-09-5, Sulfur dioxide, miscellaneous 7446-11-9, Sulfur trioxide, miscellaneous 7446-14-2, Lead sulfate 7446-18-6, Thallium sulfate 7446-70-0, Aluminum chloride (AlCl3), miscellaneous 7487-94-7, Mercuric chloride, miscellaneous 7488-56-4, Selenium disulfide 7521-80-4, Butyltrichlorosilane 7550-45-0, Titanium tetrachloride, miscellaneous 7570-26-5, 1,2-Dinitroethane 7572-29-4, Dichloroacetylene 7578-36-1 7580-67-8, Lithium hydride 7601-89-0, Sodium perchlorate 7601-90-3, Perchloric acid, miscellaneous 7616-94-6, Perchloryl fluoride 7631-89-2, Sodium arsenate 7631-99-4, Sodium nitrate, miscellaneous 7632-00-0, Sodium nitrite 7632-51-1, Vanadium tetrachloride 7637-07-2, Boron trifluoride, miscellaneous 7645-25-2, Lead arsenate 7646-69-7, Sodium hydride
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
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IT 7646-78-8, Stannic chloride, miscellaneous 7646-85-7, Zinc chloride, miscellaneous 7646-93-7, Potassium hydrogen sulfate 7647-01-0, Hydrogen chloride, miscellaneous 7647-18-9, Antimony pentachloride 7647-19-0, Phosphorus pentafluoride 7664-38-2, Phosphoric acid, miscellaneous 7664-38-2D, Phosphoric acid, esters 7664-39-3, Hydrogen fluoride, miscellaneous 7664-41-7, Ammonia, miscellaneous 7664-93-9, Sulfuric acid, miscellaneous 7681-38-1, Sodium hydrogen sulfate 7681-49-4, Sodium fluoride, miscellaneous 7681-52-9, Sodium hypochlorite 7697-37-2, Nitric acid, miscellaneous 7704-34-9, Sulfur, miscellaneous 7705-07-9D, Titanium trichloride, mixts. 7705-08-0, Ferric chloride, miscellaneous 7718-98-1, Vanadium trichloride 7719-09-7, Thionyl chloride 7719-12-2, Phosphorus trichloride 7722-64-7, Potassium permanganate 7722-84-1, Hydrogen peroxide (H2O2), miscellaneous 7723-14-0, Phosphorus, miscellaneous 7726-95-6, Bromine, miscellaneous 7727-15-3, Aluminum bromide 7727-18-6, Vanadium oxytrichloride 7727-21-1, Potassium persulfate 7727-37-9, Nitrogen, miscellaneous 7727-37-9D, Nitrogen, mixts. with rare gases 7727-54-0, Ammonium persulfate 7738-94-5, Chromic acid (H2CrO4) 7756-94-7, Triisobutylene 7757-79-1, Potassium nitrate, miscellaneous 7758-01-2, Potassium bromate 7758-09-0, Potassium nitrite 7758-19-2, Sodium chlorite 7758-94-3, Ferrous chloride 7761-88-8, Silver nitrate, miscellaneous 7773-03-7, Potassium bisulfite 7775-09-9, Sodium chlorate 7775-14-6, Sodium dithionite 7778-39-4,

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Arsenic acid 7778-44-1, Calcium arsenate 7778-54-3, Calcium hypochlorite 7778-66-7 7778-74-7, Potassium perchlorate 7779-86-4, Zinc dithionite 7779-88-6, Zinc nitrate 7782-39-0, Deuterium, miscellaneous 7782-41-4, Fluorine, miscellaneous 7782-44-7, Oxygen, miscellaneous 7782-44-7D, Oxygen, mixts. with rare gases 7782-49-2, Selenium, miscellaneous 7782-50-5, Chlorine, miscellaneous 7782-65-2, Germane 7782-78-7, Nitrosylsulfuric acid 7782-79-8D, Hydrazoic acid, copper complexes 7782-99-2, Sulfurous acid, miscellaneous 7783-06-4, Hydrogen sulfide, miscellaneous 7783-07-5, Hydrogen selenide (H2Se) 7783-08-6, Selenic acid 7783-33-7 7783-41-7, Oxygen difluoride 7783-54-2, Nitrogen trifluoride 7783-56-4, Antimony trifluoride 7783-60-0, Sulfur tetrafluoride 7783-61-1, Silicon tetrafluoride 7783-66-6, Iodine pentafluoride 7783-70-2, Antimony pentafluoride 7783-79-1, Selenium hexafluoride 7783-80-4, Tellurium hexafluoride 7783-81-5, Uranium hexafluoride 7783-82-6, Tungsten hexafluoride 7783-91-7, Silver chlorite 7784-08-9 7784-21-6, Aluminum hydride 7784-30-7, Aluminum phosphate 7784-42-1, Arsine 7784-46-5, Sodium arsenite 7786-30-3D, Magnesium chloride (MgCl2), mixt. with chlorates 7787-36-2, Barium permanganate 7787-41-9, Barium selenate 7787-71-5, Bromine trifluoride 7788-97-8, Chromic fluoride 7789-09-5, Ammonium dichromate 7789-18-6, Cesium nitrate 7789-21-1, Fluorosulfonic acid 7789-23-3, Potassium fluoride 7789-29-9, Potassium bifluoride 7789-30-2, Bromine pentafluoride 7789-38-0, Sodium bromate 7789-59-5, Phosphorus oxybromide 7789-60-8, Phosphorus tribromide 7789-61-9, Antimony tribromide 7789-69-7, Phosphorus pentabromide 7789-78-8, Calcium hydride 7790-59-2 7790-69-4, Lithium nitrate 7790-91-2, Chlorine trifluoride 7790-93-4, Chloric acid 7790-94-5,
Chlorosulfonic
acid 7790-98-9, Ammonium perchlorate 7790-99-0, Iodine monochloride 7791-10-8, Strontium chlorate 7791-23-3, Selenium oxychloride 7791-25-5, Sulfuryl chloride 7791-27-7, Disulfuryl chloride
7803-51-2,
Phosphine 7803-52-3, Stibine 7803-54-5, Magnesium diamide
7803-55-6,
Ammonium metavanadate 7803-57-8, Hydrazine hydrate 7803-62-5, Silane, miscellaneous 7803-63-6, Ammonium hydrogen sulfate 8004-09-9 8006-19-7, Amatol 8006-28-8, Soda lime 8007-56-5, Nitrohydrochloric acid 8007-58-7 8012-74-6, London Purple 8014-95-7, Fuming sulfuric acid 8049-17-0, Ferrosilicon 8050-88-2, Celluloid 8063-77-2 8065-53-0, Hexolite 8066-33-9, Pentolite 8070-50-6 9003-53-6, Polystyrene 9004-70-0, Collodion 9056-38-6, Nitrostarch 9080-17-5, Ammonium polysulfide 10022-31-8, Barium nitrate 10024-97-2, Nitrogen oxide (N2O), properties 10025-78-2, Trichlorosilane 10025-85-1, Nitrogen trichloride 10025-87-3, Phosphorus oxychloride 10025-91-9, Antimony trichloride 10026-04-7, Silicon tetrachloride 10026-11-6, Zirconium tetrachloride 10026-13-8, Phosphorus pentachloride 10031-13-7 10031-87-5, 2-Ethylbutyl acetate 10034-81-8, Magnesium perchlorate 10034-85-2, Hydrogen iodide 10035-10-6, Hydrogen bromide, miscellaneous 10039-54-0, Hydroxylamine sulfate 10042-76-9, Strontium nitrate 10045-94-0, Mercuric nitrate 10049-04-4, Chlorine dioxide 10099-74-8, Lead nitrate 10101-50-5 10102-06-4, Uranyl nitrate 10102-12-2, Selenium nitride 10102-18-8, Sodium selenite 10102-43-9, Nitric oxide, miscellaneous 10102-44-0, Nitrogen dioxide, miscellaneous 10102-49-5, Ferric arsenate 10102-50-8, Ferrous arsenate 10103-50-1 10118-76-0 10124-37-5, Calcium nitrate 10124-48-8, Mercury ammonium chloride 10124-50-2, Potassium arsenite 10137-74-3, Calcium chlorate 10192-29-7, Ammonium chlorate 10241-05-1, Molybdenum pentachloride 10256-53-8, Methanamine, compd. with trinitromethane, miscellaneous 10294-33-4, Boron tribromide 10294-34-5, Boron trichloride 10306-83-9

L12 ANSWER 2 OF 3 CA COPYRIGHT 2007 ACS on STN (Continued)
10326-21-3, Magnesium chlorate 10326-24-6 10361-95-2, Zinc chlorate 10377-60-3, Magnesium nitrate 10377-66-9, Manganese nitrate 10415-75-5, Mercurous nitrate 10421-48-4, Ferric nitrate 10431-47-7 10544-63-5, Ethyl crotonate 11069-19-5, Dichlorobutene 11071-47-9, Isooctene 11099-22-2 11105-16-1, Zirconium hydride 11122-26-2 11135-81-2 11138-49-1, Sodium aluminate 11140-68-4, Titanium hydride 12001-29-5, Chrysotile 12002-19-6, Mercury nucleate 12002-48-1, Trichlorobenzene 12030-88-5, Potassium superoxide 12031-80-0, Lithium peroxide 12033-49-7, Nitrogen trioxide
12034-12-7,
Sodium superoxide 12057-74-8, Magnesium phosphide (Mg3P2) 12125-01-8, Ammonium fluoride 12135-76-1, Ammonium sulfide 12136-15-1, Mercury nitride 12164-94-2, Ammonium azide 12167-20-3, Nitrocresol 12172-67-7, Actinolite 12401-70-6, Potassium monoxide 12401-86-4, Sodium monoxide 12427-38-2, Maneb 12440-42-5, Tin phosphide (Sn3P4) 12504-16-4, Strontium phosphide (Sr3P2) 12627-52-0, Antimony sulfide 12627-52-0D, Antimony sulfide, mixt. with chlorates 12640-89-0,
Selenium
oxide 12653-71-3, Mercury oxide 12737-18-7, Calcium silicide 12751-03-0, Cordite 12771-08-3, Sulfur chloride 12789-46-7, Amyl acid phosphate 13092-75-6, Silver acetylide 13138-45-9 13225-10-0, α-Methylglucoside tetranitrate 13319-75-0, Boron trifluoride dihydrate 13410-01-0, Sodium selenate 13424-46-9, Lead azide 13426-91-0, Cupriethylenediamine 13437-80-4, Mercuric arsenate 13444-85-4, Nitrogen triiodide 13446-10-1, Ammonium permanganate 13446-48-5, Ammonium nitrite 13450-97-0, Strontium perchlorate 13453-30-0, Thallium chlorate 13463-39-3, Nickel carbonyl 13463-40-6, Iron pentacarbonyl 13464-33-0, Zinc arsenate 13464-58-9D, Arsenous acid, copper complexes 13465-73-1, Bromosilane 13465-95-7, Barium perchlorate 13472-08-7 13473-90-0, Aluminum nitrate
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(packaging and transport of, stds. for)
IT 13477-00-4, Barium chlorate 13477-10-6, Barium hypochlorite 13477-36-6, Calcium perchlorate 13520-83-7, Uranyl nitrate hexahydrate 13537-32-1, Fluorophosphoric acid 13548-38-4, Chromium nitrate 13597-54-1, Zinc selenate 13597-99-4, Beryllium nitrate 13598-36-2, Phosphonic acid 13637-63-3, Chlorine pentafluoride 13637-76-8, Lead perchlorate 13718-59-7 13746-89-9, Zirconium nitrate 13762-51-1, Potassium borohydride 13766-44-4, Mercury sulfate 13769-43-2, Potassium metavanadate 13770-96-2, Sodium aluminum hydride 13774-25-9 13779-41-4, Difluorophosphoric acid 13780-03-5, Calcium bisulfite 13823-29-5, Thorium nitrate 13840-33-0, Lithium hypochlorite 13840-33-0D, Lithium hypochlorite, mixts. 13843-59-9, Ammonium bromate 13863-88-2, Silver azide 13967-90-3, Barium bromate 13973-87-0, Bromine azide 13973-88-1, Chlorine azide 13987-01-4, Tripropylene 14014-86-9 14019-91-1, Calcium selenate 14293-73-3 14448-38-5, Hyponitrous acid 14519-07-4, Zinc bromate 14519-17-6, Magnesium bromate 14546-44-2, Hydrazine azide 14567-73-8, Tremolite 14644-61-2, Zirconium sulfate 14666-78-5, Diethylperoxydicarbonate 14674-72-7, Calcium chlorite 14696-82-3, Iodine azide (I(N3)) 14977-61-8 15195-06-9 15245-44-0, Lead trinitroresorcinate 15347-57-6, Lead acetate 15457-98-4 15512-36-4, Calcium dithionite 15545-97-8, 2,2'-Azodi(2,4-dimethyl-4-methoxyvaleronitile) 15598-34-2, Pyridine perchlorate 15718-71-5, Ethylenediamine diperchlorate 15825-70-4, Mannitol hexanitrate 15875-44-2, Methylamine perchlorate 16215-49-9, Di-n-butyl peroxydicarbonate 16229-43-9, Vanadyl sulfate 16339-86-9 16646-35-8 16721-80-5, Sodium hydrosulfide 16753-36-9, Copper acetylide 16853-85-3, Lithium aluminum hydride 16871-71-9,
Zinc

L12 ANSWER 2 OF 3 CA COPYRIGHT 2007 ACS on STN (Continued)
fluorosilicate 16871-90-2, Potassium fluorosilicate 16872-11-0
16893-85-9, Sodium fluorosilicate 16901-76-1, Thallium nitrate
16919-19-0, Ammonium fluorosilicate 16940-66-2, Sodium borohydride
16940-81-1, Hexafluorophosphoric acid 16941-12-1, Chloroplatinic acid
16949-15-8, Lithium borohydride 16949-65-8, Magnesium fluorosilicate
16961-83-4, Fluorosilicic acid 16962-07-5, Aluminum borohydride
17014-71-0, Potassium peroxide 17068-78-9, Anthophyllite 17462-58-7,
sec-Butyl chloroformate 17639-93-9, Methyl-2-chloropropionate
17702-41-9, Decaborane 17861-62-0 18130-44-4, Titanium
sulfate 18414-36-3 18810-58-7, Barium azide 19159-68-3
19287-45-7,
Diborane 19287-45-7D, Diborane, mixts. 19624-22-7, Pentaborane
20062-22-0 20236-55-9, Barium styphnate 20600-96-8 20816-12-0,
Osmium tetroxide 20820-44-4 20859-73-8, Aluminum phosphide
21351-79-1, Cesium hydroxide (Cs(OH)) 21569-01-7 21723-86-4
21985-87-5, Pentanitroaniline 22128-62-7, Chloromethylchloroformate
22750-93-2, Ethyl perchlorate 22751-24-2 22826-61-5 23414-72-4,
Zinc
permanganate 23745-86-0, Potassium fluoroacetate 24167-76-8, Sodium
phosphide 24468-13-1, 2-Ethylhexylchloroformate 24884-69-3
25013-15-4, Vinyl toluene 25109-57-3 25134-21-8 25136-55-4,
Dimethyldioxane 25154-42-1, Chlorobutane 25154-54-5, Dinitrobenzene
25155-15-1, Cymene 25167-20-8, Tetrabromoethane 25167-67-3, Butylene
25167-70-8, Diisobutylene 25167-80-0, Chlorophenol 25168-05-2,
Chlorotoluene 25265-68-3, Methyltetrahydrofuran 25321-14-6,
Dinitrotoluene 25322-01-4, Nitropropane 25322-20-7, Tetrachloroethane
25323-30-2, Dichloroethylene 25339-56-4, Heptene 25340-17-4,
Diethylbenzene 25377-72-4, n-Amylene 25496-08-6, Fluorotoluene
25497-28-3, Difluoroethane 25497-29-4, Chlorodifluoroethane
25513-64-8
25550-53-2 25550-55-4, Dinitrosobenzene 25550-58-7, Dinitrophenol
25550-58-7D, Dinitrophenol, salts 25567-67-3, Chlorodinitrobenzene
25567-68-4, Chloronitrotoluene 25639-42-3, Methylcyclohexanol
25721-38-4, Lead picrate 25917-35-5, Hexanol 26134-62-3, Lithium
nitride 26140-60-3D, Terphenyl, halo derivs. 26249-12-7,
Dibromobenzene 26471-56-7, Dinitroaniline 26471-62-5, Toluene
diisocyanate 26506-47-8, Copper chlorate 26571-79-9 26618-70-2
26628-22-8, Sodium azide 26638-19-7, Dichloropropane 26645-10-3
26760-64-5, Isopentene 26762-93-6 26914-02-3, Iodopropane
26915-12-8, Toluidine 26952-23-8, Dichloropropene 26952-42-1,
Trinitroaniline 27134-26-5, Chloroaniline 27134-27-6, Dichloroaniline
27137-85-5, Dichlorophenyltrichlorosilane 27152-57-4 27176-87-0,
Dodecylbenzenesulfonic acid 27195-67-1, Dimethylcyclohexane
27215-10-7
27236-46-0, Isohexene 27254-36-0, Nitronaphthalene 27458-20-4,
Butyltoluene 27978-54-7, Hydrazine perchlorate 27986-95-4
27987-06-0, Trifluoroethane 28260-61-9, Trinitrochlorobenzene
28300-74-5, Antimony potassium tartrate 28324-52-9, Pinane
hydroperoxide
28479-22-3 28653-16-9 28679-16-5, Trimethylhexamethylenediisocyanate
28805-86-9, Butylphenol 29191-52-4, Anisidine 29306-57-8
29790-52-1,
Nicotine salicylate 29903-04-6 29965-97-7, Cyclooctadiene
30236-29-4, Sucrose octanitrate 30525-89-4, Paraformaldehyde
30553-04-9, Naphthylthiourea 30586-10-8, Dichloropentane 30586-18-6,

L12 ANSWER 2 OF 3 CA COPYRIGHT 2007 ACS on STN (Continued)
Pentamethylheptane 31058-64-7 31212-28-9, Nitrobenzenesulfonic acid
33453-96-2 33864-17-4 34216-34-7, Trimethylcyclohexylamine
35296-72-1, Butanol 35860-50-5, Trinitrobenzoic acid 35860-51-6,
Dinitroresorcinol 35884-77-6, Xylyl bromide 36472-34-1, Chloropropene
37020-93-2, Mercury cyanide (Hg(CN)) 37187-22-7, Acetyl acetone
peroxide
37206-20-5, Methyl isobutyl ketone peroxide 37273-91-9, Metaldehyde
37320-91-5, Mercury iodide 37368-10-8, Aluminum vanadium oxide
38139-71-8, Bromide chloride 38232-63-2, Mercurous azide 38483-28-2,
Methylene glycol dinitrate 39377-49-6, Copper cyanide 39377-56-5,
Lead
sulfide 39404-03-0, Magnesium silicide 39409-64-8, TVOPA 39432-81-0
39455-80-6, Ammonium sodium vanadium oxide 40058-87-5,
Isopropyl-2-chloropropionate 41195-19-1 41587-36-4,
Chloronitroaniline
42296-74-2, Hexadiene 43133-95-5, Methylpentane 50815-73-1
50874-93-6 51006-59-8 51023-22-4, Trichlorobutene 51064-12-1
51312-23-3, Mercury bromide 51317-24-9, Lead nitroresorcinate
51325-42-9, Copper selenite 51845-86-4, Ethyl borate 52181-51-8
53014-37-2, Tetranitroaniline 53408-91-6, Mercury thiocyanate
53422-49-4 53569-62-3 53839-08-0 53906-68-6 54141-09-2,
1,4,-Butynediol 54413-15-9, Tritonal 54727-89-8 54958-71-3
55510-04-8, Dinitroglycoluril 55810-17-8
RL: ADV (Adverse effect, including toxicity); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(packaging and transport of, stds. for)

L12 ANSWER 3 OF 3 CA COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 51:35047 CA
ORIGINAL REFERENCE NO.: 51:6704g-i,6705a-c
TITLE: Substituted pyridines
INVENTOR(S): Mahan, John E.
PATENT ASSIGNEE(S): Phillips Petroleum Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2775596		19561225	US 1952-315837	19521020

GI For diagram(s), see printed CA Issue.
AB New catalysts are reported for the condensation of carbonyl compds. with NH3 in the preparation of alkylpyridines useful as intermediates for pyridine derivs. with unsatd. side chains, which are in turn intermediates for synthetic rubber. An electrically heated 1.4-l. stainless steel bomb was charged with 170 g. paraldehyde (I), 173 g. NH3 in 211 cc. H2O (molar ratio NH3-I = 7.91), and 0.18 mole metal fluoride as catalyst, sealed, the air replaced by N, the bomb heated 3 hrs. at 490-500°F. while shaken by an electrically driven rocker, the excess NH3 allowed to escape, the remaining mixture extracted with C6H6, and the extract fractionated (metal in the fluoride catalyst used, and yields (mole-%) of picolines and 2-methyl-3-ethylpyridine given): no catalyst, 2.6, 56.3; Sb, 1.5, 76.8; Cu (cupric), 2.8, 71.8; Bi, 1.8, 71.0; Zn, 1.8, 69.8; Fe (ferric), 2.3, 69.8; Ba, 2.6, 69.5; Ag, 2.8, 61.9; Al, 3.5, 61.8; Ti, 1.7, 60.8. Thus, all the catalysts increase the yield over the control run, and those preferred are the fluorides (or fluorides associated with H2F2) of metals in groups Ib and II-VIII of the periodic table. Suitable carbonyl compds. other than I are MeCH:CHCHO, PhCH: CHBz, PhCH(CH2Bz)2 (II), MeCH:CHAc (III), p-ClC6H4CH(CH2Bz)2, p-MeOC6H4CH(CH2Bz)2, OC.O.CH2.CH2.CHAc, cyclopentanone, tetrahydropyrone, and β-cyclohexylpropionaldehyde, or mixts. of BzH and AcPh, II and AcPh, BzH and PhCH2Bz, III and AcPh, or III and Me2 CO. Most suitable are aliphatic aldehydes or ketones with 2 α-H atoms. The catalyst amount may vary from 0.2-10% by weight of the carbonyl compound used, the molar ratio NH3-carbonyl compound from 1-12, the reaction temperature from 300 to 600°F., the time of heating from 5 min. to 5 hrs. The NH3 may be liquid or in aqueous solution Emulsifying agents may be used in amts. from 0.1-5% by weight Water-soluble metal phosphate glasses may be added to the reaction mixture as synergists in aqueous solution or as solids in amts. from 0.05-10% by weight of the carbonyl compound
AB New catalysts are reported for the condensation of carbonyl compds. with NH3 in the preparation of alkylpyridines useful as intermediates for pyridine derivs. with unsatd. side chains, which are in turn intermediates for synthetic rubber. An electrically heated 1.4-l. stainless steel bomb was charged with 170 g. paraldehyde (I), 173 g. NH3 in 211 cc. H2O (molar ratio NH3-I = 7.91), and 0.18 mole metal fluoride as catalyst, sealed, the air replaced by N, the bomb heated 3 hrs. at 490-500°F. while shaken by an electrically driven rocker, the excess NH3 allowed to escape, the remaining mixture

L12 ANSWER 3 OF 3 CA COPYRIGHT 2007 ACS on STN (Continued)
extd. with C6H6, and the ext. fractionated (metal in the fluoride catalyst used, and yields (mole-%) of picolines and 2-methyl-3-ethylpyridine given): no catalyst, 2.6, 56.3; Sb, 1.5, 76.8; Cu (cupric), 2.8, 71.8; Bi, 1.8, 71.0; Zn, 1.8, 69.8; Fe (ferric), 2.3, 69.8; Ba, 2.6, 69.5; Ag, 2.8, 61.9; Al, 3.5, 61.8; Ti, 1.7, 60.8. Thus, all the catalysts increase the yield over the control run, and those preferred are the fluorides (or fluorides assocd. with H2F2) of metals in groups Ib and II-VIII of the periodic table. Suitable carbonyl compds. other than I are MeCH:CHCHO, PhCH: CHBz, PhCH(CH2Bz)2 (II), MeCH:CHAc (III), p-ClC6H4CH(CH2Bz)2, p-MeOC6H4CH(CH2Bz)2, OC.O.CH2.CH2.CHAc, cyclopentanone, tetrahydropyrone, and β-cyclohexylpropionaldehyde, or mixts. of BzH and AcPh, II and AcPh, BzH and PhCH2Bz, III and AcPh, or III and Me2 CO. Most suitable are aliphatic aldehydes or ketones with 2 α-H atoms. The catalyst amt. may vary from 0.2-10% by wt. of the carbonyl compd. used, the molar ratio NH3-carbonyl compd. from 1-12, the reaction temp. from 300 to 600°F., the time of heating from 5 min. to 5 hrs. The NH3 may be liquid or in aq. soln. Emulsifying agents may be used in amts. from 0.1-5% by wt. Water-sol. metal phosphate glasses may be added to the reaction mixt. as synergists in aq. soln. or as solids in amts. from 0.05-10% by wt. of the carbonyl compd.
IT Condensation, chemical
(of ammonia with carbonyl compds.)
IT Carbonyl compounds
(reactions of, with NH3)
IT 104-90-5P, 2-Picoline, 5-ethyl- 1333-41-1P, Picoline
RL: PREP (Preparation)
(manufacture of)
IT 7664-41-7, Ammonia
(reactions of, with carbonyl compds.)

An alternative to view hit terms when display exceeds KWIC processing limits is to use HIT display format.

```
=> d his

     (FILE 'HOME' ENTERED AT 11:22:35 ON 11 JUN 2007)

     FILE 'CASREACT' ENTERED AT 11:22:50 ON 11 JUN 2007
L1                STRUCTURE UPLOADED
L2              5 S L1 SAM
L3              0 S L2 AND CATALYST

     FILE 'CA' ENTERED AT 11:24:03 ON 11 JUN 2007
L4              0 S PICOLINE/PROD
L5              0 S PICOLINE/PRO
L6          14074 S PICOLINE
L7         200820 S CARBONYL?
L8         964462 S AMMONIA? OR NH?
L9          17169 S L7 AND L8
L10           130 S L9 AND  L6
L11        625653 S TI OR TITANIUM?
L12             3 S L11 AND L10

=>

---Logging off of STN---



=>
Executing the logoff script...


=> LOG Y

 * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:27:33 ON 11 JUN 2007

=> file casreact

=> s l1 full
FULL SEARCH INITIATED 11:28:13 FILE 'CASREACT'
SCREENING
SCREENING COMPLETE -    994928 REACTIONS TO VERIFY FROM    65642 DOCUMENTS

 77.8% DONE  774500 VERIFIED   10264 HIT RXNS                        854 DOCS

 98.9% DONE  984251 VERIFIED   12540 HIT RXNS                       1079 DOCS

100.0% DONE  994928 VERIFIED   12914 HIT RXNS                       1094 DOCS
SEARCH TIME: 00.00.59

L2            1094 SEA SSS FUL L1 ( 12914 REACTIONS)

=> d l1
L1 HAS NO ANSWERS
L1                STR
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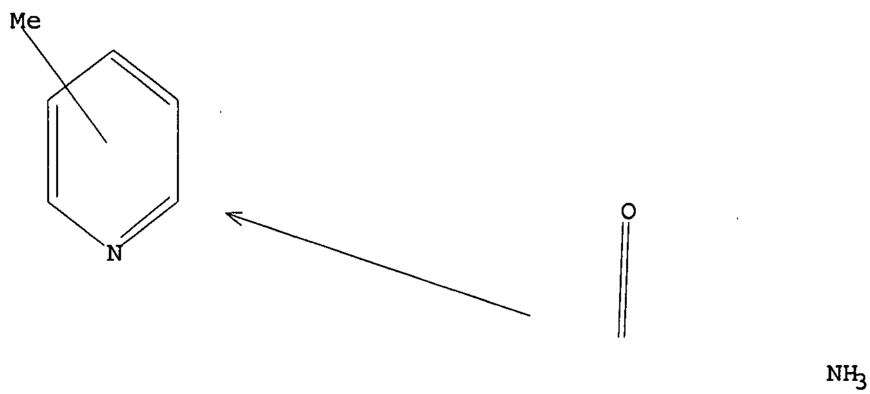

Structure attributes must be viewed using STN Express query preparation.

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=> s l2 and (ti? or titanium?)
        138117 TI?
          9203 TITANIUM?
L3         255 L2 AND (TI? OR TITANIUM?)

=> s l3 and (gas phas?)
         12988 GAS
         29456 PHAS?
          3966 GAS PHAS?
                 (GAS(W)PHAS?)
L4          12 L3 AND (GAS PHAS?)

=> d ibib abs fhit 1-12
```

L4 ANSWER 1 OF 12 CASREACT COPYRIGHT 2007 ACS on STN

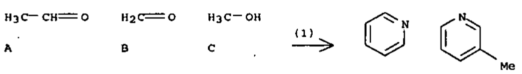
ACCESSION NUMBER: 146:251736 CASREACT
TITLE: A catalytic cyclocondensation process for preparing pyridine and alkyl-substituted pyridines from aldehydes and/or ketones with ammonia
INVENTOR(S): Singh, Shailendra Kumar; Tiwari, Neeraj; Kulshreshtha, Vimaldeep; Agarwal, Ashutosh
PATENT ASSIGNEE(S): Jubilant Organosys Ltd., India
SOURCE: Indian, 32pp.
CODEN: INXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 193364	A1	20040717	IN 2002-DE26	20020115

PRIORITY APPLN. INFO.: IN 2002-DE26 20020115

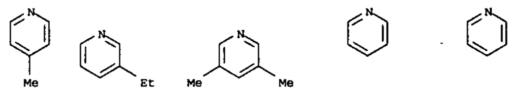
AB A process for preparing pyridine (e.g., pyridine) and alkyl-substituted pyridines comprises the cyclocondensation reaction of a C1-5 aldehyde (e.g., acetone and formalin) and/or a C3-5 ketone with ammonia in the gaseous phase in the presence of a catalyst in a fluidized or otherwise movable bed reactor at 350-550°/0.1-5 atm, the catalyst being a mixture of crystalline silica-alumina zeolite catalyst and amorphous silica-alumina catalyst in a weight ratio of 80:20 to 98:2, the amorphous or crystalline silica-alumina zeolite catalyst optionally being modified by exchanging with elements (e.g., Pd) and being maintained in the reactor at anytime during the reaction.

RX(1) OF 1 A + B + C ===> D + E + F + G + H + I + J



A B C D E

L4 ANSWER 1 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



F G H I J

RX(1)
RCT A 75-07-0, B 50-00-0, C 67-56-1
RGT K 7664-41-7 NH3, L 7732-18-5 Water
PRO D 110-86-1, E 108-99-6, F 108-89-4, G 536-78-7, H 591-22-0, I 27175-64-0, J 29611-84-5
CON 10 hours, 450 deg C
NTE Zeolite catalyst comprised ZSM-5 in a silica-alunima clay matrix, gas phase, thermal

L4 ANSWER 2 OF 12 CASREACT COPYRIGHT 2007 ACS on STN

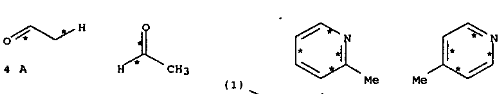
ACCESSION NUMBER: 143:117138 CASREACT
TITLE: Catalyst for synthesis of 2- and 4-picolines, process for preparing 2- and 4-picoline and process for preparing the catalyst
INVENTOR(S): Dutta, Pashupati; Roy, Subhash Chandra; Roy, Shyam Kishor; Goswami, Tarun Kanti
PATENT ASSIGNEE(S): Council of Scientific & Industrial Research, India
SOURCE: PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063389	A1	20050714	WO 2003-IN467	20031231
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2552158	A1	20050714	CA 2003-2552158	20031231
AU 2003300723	A1	20050721	AU 2003-300723	20031231
EP 1708811	A1	20061011	EP 2003-819218	20031231
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1886195	A	20061227	CN 2003-80110944	20031231
IN 2004DN00489	A	20060310	IN 2004-DN489	20040227
US 2005209458	A1	20050922	US 2004-806063	20040322

PRIORITY APPLN. INFO.: WO 2003-IN467 20031231

AB Title catalyst comprises a heteropoly acid selected from the group consisting of silicotungstic acid, phosphotungstic acid, phosphomolybdic acid and vanadotungstic acid provided on a support. The support is selected from the group consisting of silica gel, alumina, silica-alumina, clays and montmorillonite. The invention also provides a process for the preparation thereof and use thereof for the synthesis of 2- and 4-picolines useful as intermediates for pharmaceuticals and agrochems.

RX(1) OF 3 6 A ===> B + C



4 A 2 A B C

L4 ANSWER 2 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(1)

STAGE(1)
RGT D 7782-44-7 O2
CAT 7631-86-9 SiO2, 1343-93-7 Tungstate(3-), tetracosa-μ-oxododecaoxo[μ12-[phosphato(3-)-κO:κO:κO:κO':κO':κO':.kappa.O'':κO'':κO'':κO''':κO''':.kappa.O''']]dodeca-, hydrogen (1:3)
SOL 7732-18-5 Water
CON SUBSTAGE(1) 1 hour, 200 - 250 deg C
SUBSTAGE(2) 1 hour, 400 deg C
SUBSTAGE(3) 400 deg C -> room temperature

STAGE(2)
RCT A 75-07-0
RGT E 7664-41-7 NH3
CON 2 hours, 380 deg C

PRO B 109-06-8, C 108-89-4
NTE gas phase, solid-supported catalyst, catalyst prepd. in situ, 50-60% conversion

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 12 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:43780 CASREACT
TITLE: Catalytic process for production of pyridine and picolines from ammonia and aldehydes or ketones using MFI zeolites which contain zirconium or tin
INVENTOR(S): Agarwal, Ashutosh; Verma, Pradeep Kumar; Singh, Kumar Samir; Joshi, Praphulla Narahar; Chaphekar, Gopal Moreshwar; Niphadkar, Prashant Suresh; Kumar, Rajiv
PATENT ASSIGNEE(S): Council of Scientific & Industrial Research, India; Jubilant Organosys Limited
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054197	A1	20050616	WO 2003-IN385	20031205

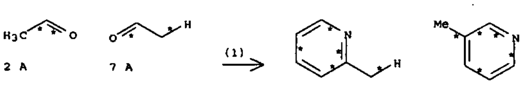
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AU 2003304586	A1	20050624	AU 2003-304586	20031205
US 2005209457	A1	20050922	US 2004-806061	20040322

PRIORITY APPLN. INFO.: WO 2003-IN385 20031205

AB A single-step catalytic process for the production of pyridine and picolines (e.g., α-picoline and γ-picoline) from a gas-phase mixture of a carbonyl compound (e.g., acetaldehyde) and ammonia in the presence of zeolite catalyst with an MFI zeolite containing Si and Zr and/or Sn is described.

RX(1) OF 2 9 A ===> B + C + D



2 A 7 A B YIELD 51% C YIELD 25%

L4 ANSWER 3 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

D
YIELD 1%

RX(1) RCT A 75-07-0
RGT E 7664-41-7 NH3
PRO B 109-06-8, C 108-99-6, D 110-86-1
CAT 7440-67-7 Zr
SOL 7732-18-5 Water
CON 390 - 400 deg C
NTE gas phase, regioselective, down-flow fixed-bed reactor used, optimized on catalyst, Pb/ZrS-1B catalyst used

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 12 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:113907 CASREACT
TITLE: Catalytic process for the production of pyridine and picolines from ammonia and carbonyl compounds
INVENTOR(S): Kumar, Rajiv; Joshi, Praphulla Narahar; Chapekar, Gopal Moreshwar; Niphadkar, Prashant Suresh; Agarwal, Ashutosh; Verma, Pradeep Kumar; Singh, Kumar Samir
PATENT ASSIGNEE(S): Council of Scientific and Industrial Research, India; Jubilant Organosys Ltd.
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005000816	A1	20050106	WO 2003-IN465	20031231

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

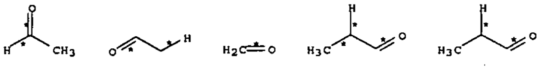
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005131235	A1	20050616	US 2003-731440	20031210
AU 2003300721	A1	20050113	AU 2003-300721	20031231
EP 1648869	A1	20060426	EP 2003-817293	20031231

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.: IN 2003-DE853 20030627
WO 2003-IN465 20031231

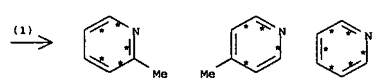
AB A process for the preparation of pyridine and/or picolines (e.g., a mixture of α-picoline and γ-picoline) is described which comprises contacting a mixture of a carbonyl compound (e.g., acetaldehyde) with ammonia in the presence of a surface-passivated titanium silicate catalyst in gas phase at 300-500°/1-10 bar, a gas space velocity of 300-3000 h-1, condensing and separating the products by conventional methods and if desired, further purifying the product using conventional methods.

RX(1) OF 1 2 A + 8 B + 2 C ===> D + E + F



A A 8 B C C

L4 ANSWER 4 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



D E F

RX(1) RCT A 75-07-0, B 50-00-0, C 123-38-6
RGT G 7664-41-7 NH3
PRO D 109-06-8, E 108-89-4, F 110-86-1
CAT 42613-21-8D Silicic acid, titanium salt
CON 390 - 400 deg C
NTE flow system, gas phase, optimization study, thermal, optimized on catalyst and catalyst crystal size, down flow fixed bed reactor was used

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 12 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:424117 CASREACT

TITLE: Preparation of pyridine bases from aliphatic carbonyl compounds and ammonia, and zeolite compositions and catalysts for the process

INVENTOR(S): Yamamoto, Kohei; Kimura, Manabu

PATENT ASSIGNEE(S): Koei Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

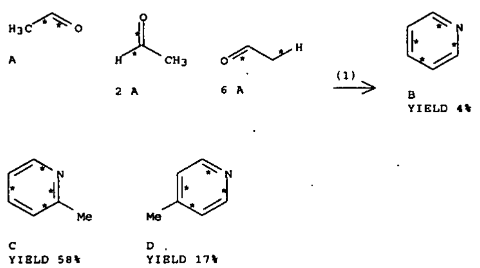
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004331555	A	20041125	JP 2003-128774	20030507
PRIORITY APPLN. INFO.:			JP 2003-128774	20030507

AB Pyridine bases are prepared by contacting aliphatic aldehydes and/or ketones with NH_3 in gas phase in the presence of catalysts prepared by molding TiO_2 binder and zeolites containing B and Si. Thus, NH_3 and MeCHO were passed at 450° through a column packed with MFI zeolite containing TiO_2 and Pb, which was regenerated with steam every 24 h. The materials were supplied over 30 h to give pyridine, α-picoline, and γ-picoline with 2.7, 60.4, and 15.5% yield, vs. 3.9, 57.9, and 16.5%, 126 h later.

RX(1) OF 1 9 A ===> B + C + D



RX(1) RCT A 75-07-0
RGT E 7664-41-7 NH3
PRO B 110-86-1, C 109-06-8, D 108-89-4

L4 ANSWER 5 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
CON 126 hours, 450 deg C
NTE thermal, Lead Borosilicate zeolites used, alternative prepn. shown

L4 ANSWER 6 OF 12 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:93925 CASREACT

TITLE: A process for the production of β-picoline and pyridine simultaneously by catalytic aminocyclisation reaction of acetaldehyde formaldehyde & ammonia

INVENTOR(S): Sharma, Krishnadeo Prasad; Roy, Sisir Kumar; Goswami, Tarun Kanti

PATENT ASSIGNEE(S): Council of Scientific and Industrial Research, India

SOURCE: Indian, 7 pp.
CODEN: INXXAP

DOCUMENT TYPE: Patent

LANGUAGE: English

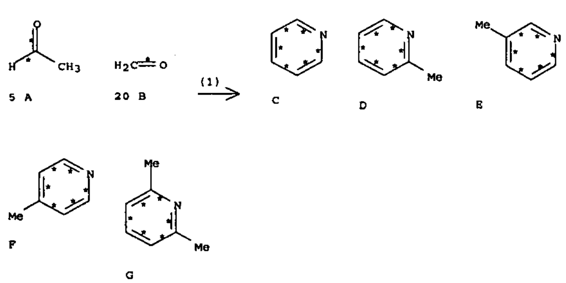
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 179006	A1	19970809	IN 1992-DE830	19920916
PRIORITY APPLN. INFO.:			IN 1992-DE830	19920916

AB A process for the production of β-picoline and pyridine simultaneously by catalytic aminocyclization reaction of acetaldehyde, formaldehyde and ammonia in vapor phase is reported. This invention comprises passing acetaldehyde, formaldehyde and ammonia through a catalyst crystalline silico alumina (Si:Al = 88:12%) impregnated with 5-10% of oxides of Zn or Cd at a temperature in the range of 350-500°C, at a contact time between 2-5 s. Pyridine and β-picoline are separated by cooling in ice-salt mixture The unreacted acetaldehyde and formaldehyde can be recycled.

RX(1) OF 1 5 A + 20 B ===> C + D + E + F + G



RX(1) RCT A 75-07-0, B 50-00-0
RGT H 7664-41-7 NH3

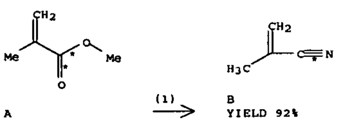
L4 ANSWER 6 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
PRO C 110-86-1, D 109-06-8, E 108-99-6, F 108-89-4, G 108-48-5
CON 2 - 3 seconds, 365 - 385 deg C
NTE zeolite catalyst bed was calcined before reaction, gas phase

L4 ANSWER 7 OF 12 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 137:247610 CASREACT
TITLE: Preparation of nitriles from esters
INVENTOR(S): Koji, Takayuki; Miura, Hiroshi; Nishimoto, Yoshihiro
PATENT ASSIGNEE(S): Koei Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002284753	A	20021003	JP 2001-85177	20010323

PRIORITY APPLN. INFO.: JP 2001-85177 20010323
AB Nitriles are prepared by reaction of carboxylic acid esters with ammonia in the presence of titania or zirconia. Thus, reaction of Me methacrylate with ammonia in the presence of titania at 300° gave 92.6% methacrylonitrile.

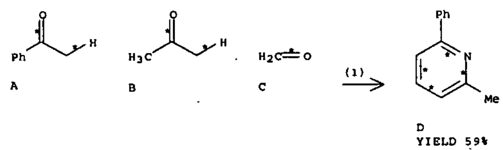
RX(1) OF 2 A ===> B



RX(1) RCT A 80-62-6
RGT C 7664-41-7 NH3
PRO B 126-98-7
CAT 13463-67-7 TiO2
NTE gas phase

L4 ANSWER 8 OF 12 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 136:118357 CASREACT
TITLE: A novel single step synthesis of 2-methyl-6-phenylpyridine from non-heterocyclic compounds over molecular sieve catalysts
AUTHOR(S): Venu Gopal, D.; Srinivas, N.; Srinivas, B.; Kulkarni, S. J.; Subrahmanyam, M.
CORPORATE SOURCE: Catalysis Division, Indian Institute of Chemical Technology, Hyderabad, 500 007, India
SOURCE: Green Chemistry (2001), 3(2), 65-67
CODEN: GRCHFJ; ISSN: 1463-9262
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The industrially important 2-methyl-6-phenylpyridine is synthesized for the first time in a single step by reacting acetophenone, acetone, formaldehyde and ammonia in the vapor phase over microporous and mesoporous mol. sieve catalysts.

RX(1) OF 1 A + B + C ===> D



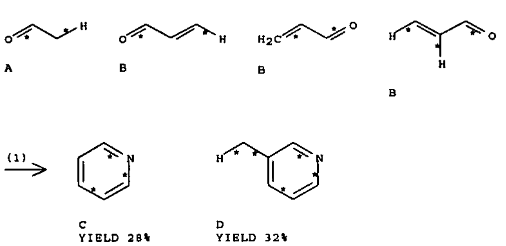
RX(1) RCT A 98-86-2, B 67-64-1, C 50-00-0
RGT E 7664-41-7 NH3
PRO D 46181-30-0
NTE green chem., green chem.-process simplification, gas phase, mol. sieves/catalyst used, mol. sieves MCM-41/catalyst used, yield depends on type of mol. sieves used,
no solvent, fixed-bed down-flow reactor used, other products also detected
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 12 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 128:75314 CASREACT
TITLE: Preparation of pyridine bases.
INVENTOR(S): Matsuoka, Kazutuki; Miki, Keiko
PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09328470	A	19971222	JP 1996-145440	19960607

PRIORITY APPLN. INFO.: JP 1996-145440 19960607
AB Pyridine bases are prepared by condensation of aliphatic aldehydes and/or ketones with NH3 in the presence of crystalline metal aluminophosphate catalysts in gas phases. A mixt containing H2C:CHCHO, CH3CHO, and NH3 (1.9:1:3.48 at mol ratio) was fed into a reactor packed with a catalysts (prepared by calcined SAPO-11 at 500° under air) at 450° and SV 370 h/r for 6 h to give 28.41% pyridine, 32.37% β-picoline, and 1.53% α-picoline.

RX(1) OF 1 A + 3 B ===> C + D



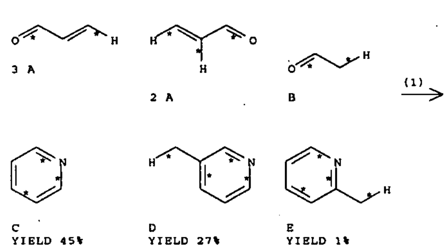
RX(1) RCT A 75-07-0, B 107-02-8
RGT E 7664-41-7 NH3
PRO C 110-86-1, D 108-99-6
NTE SAPO-11 silicoaluminophosphate zeolite catalyst

L4 ANSWER 10 OF 12 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 126:89276 CASREACT
TITLE: Preparation of pyridine bases by catalytic gas-phase reaction of aldehydes and/or ketones with ammonia
PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08333343	A	19961217	JP 1996-142175	19960513
EP 764638	A1	19970326	EP 1996-401325	19960618
EP 764638	B1	20010418		
R: BE, DE, FR, GB, IT, NL				

PRIORITY APPLN. INFO.: US 1995-481082 19950607
JP 1995-270607 19950925
JP 1996-142175 19960513
AB Claimed is a process for preparation of the title compds. by gas-phase cyclocondensation of aldehydes and/or ketones with ammonia over metal-zeolite catalysts. The title compds., useful as intermediates in the production of drugs and pesticides, are prepared in an industrial manner safely and economically. Thus, a mixture of CH2:CHCHO, MeCHO, and NH3 was reacted over HZSM-5/Ag (preparation given) at 450° for 6 h to give 45% pyridine, 27% β-picoline, and 1% α-picoline.

RX(1) OF 1 5 A + B ===> C + D + E



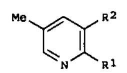
RX(1) RCT A 107-02-8, B 75-07-0
RGT F 7664-41-7 NH3
PRO C 110-86-1, D 108-99-6, E 109-06-8
CAT 7761-88-8 AgNO3
NTE 450.DEGREE. FOR 6 H; GHSV 500, HZSM-5 ALSO PRESENT AS CATALYST

L4 ANSWER 10 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 11 OF 12 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 126:47101 CASREACT
TITLE: Preparation of 3-methylpyridine derivatives by gas-phase catalytic cyclocondensation of methacrolein with carbonyl compounds and ammonia
INVENTOR(S): Uchiumi, Hiroshi; Anzai, Ryuichi
PATENT ASSIGNEE(S): Nitto Chemical Industry Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08259537	A	19961008	JP 1995-90099	19950324

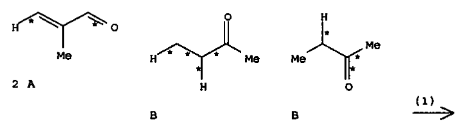
PRIORITY APPLN. INFO.: JP 1995-90099 19950324
OTHER SOURCE(S): MARPAT 126:47101
GI



I

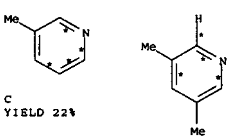
AB The title compds. (I; R1, R2 = H, C1-4 alkyl) are prepared by cyclocondensation of methacrolein with R1COCH2R2 (R1, R2 = same as above) and NH3 over catalysts SiaXbYcZdOe (X = P, B; Y = Li, Na, K, Rb, Cs, Mg, Sr, Ba, La; Z = Ce, Ti, Zr, V, Nb, etc.; a, b, c, d, e = atomic ratio; when a = 10, b = 0.2-10, c = 0-3, d = 0-5; e = number of corresponding to the formed oxide) in the presence of water steam. I are useful materials in the production of drugs, pesticides, and polymers. Thus, methacrolein was reacted with NH3 and MeCOEt over catalyst Si10P1.25B1.5O25.38 (preparation given) at 350° for 4.0 s. to give 22% I (R1 = R2 = Me) and 20% I (R1 = H, R2 = Me) resp.

RX(1) OF 1 2 A + 2 B ===> C + D



2 A B B

L4 ANSWER 11 OF 12 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



C
YIELD 22%

D
YIELD 20%

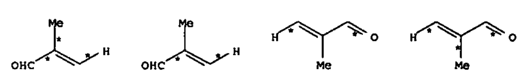
RX(1) RCT A 78-85-3, B 78-93-3
RGT E 7664-41-7 NH3
PRO C 108-99-6, D 591-22-0
CAT 184580-39-0 Silicon borate oxide phosphate (Si10(BO3)1.5O15.88(PO4)1.25)
NTE 350° for 4 s

L4 ANSWER 12 OF 12 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 126:18794 CASREACT
TITLE: Preparation of di- and trimethylpyridine using silicon-containing metal oxide as catalysts
INVENTOR(S): Uchiumi, Hiroshi; Anzai, Ryuichi; Morya, Kyoshi
PATENT ASSIGNEE(S): Nitto Chemical Industry Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

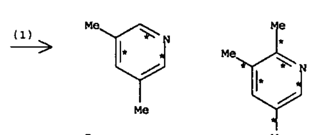
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08245589	A	19960924	JP 1995-83488	19950316

PRIORITY APPLN. INFO.: JP 1995-83488 19950316
AB The title compds. (I) are prepared by vapor-phase reaction of methacrolein with NH3 over catalysts SiaXbBcYdZeOf (X = Zr, Al, P; Y = Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba, La; Z = Ce, Ti, V, Nb, Ta, Cr, Mo, W, Mn, Re, Fe, Co, Ni, Cu, Ag, Zn, Sn, Pb, Sb, Bi, S, Te; a, b, c, d, e, f = atomic ratio; when a = 10, b = 0.2-25, c = 0-7, d = 0-3, e = 0-3; f = number of oxide) in the presence of water steam. I are useful materials in the production of drugs, pesticides, and polymers. Thus, methacrolein was reacted with NH3 over Si10P1.0B1.0O24 catalyst (preparation given) at 340 ° for 4.0 h to give 49.1% 3,5-di- and 6.9% 2,3,5-trimethylpyridine.

RX(1) OF 1 4 A ===> B + C



A A A A



B
YIELD 49%

C
YIELD 7%

RX(1) RCT A 78-85-3
RGT D 7664-41-7 NH3

```
L4   ANSWER 12 OF 12  CASREACT  COPYRIGHT 2007 ACS on STN     (Continued)
          PRO  B 591-22-0, C 695-98-7
          CAT  184375-87-9 Silicon borate oxide phosphate (Si10(BO3)O17(PO4))
          NTE  340° for 4 h; ratio of 17 : 9058 : N2 : H2O = 1 : 1 : 9 :
               2; 100% convension
```

```
=> d his

     (FILE 'HOME' ENTERED AT 11:27:33 ON 11 JUN 2007)

     FILE 'CASREACT' ENTERED AT 11:27:41 ON 11 JUN 2007
L1                STRUCTURE UPLOADED
L2           1094 S L1 FULL
L3            255 S L2 AND (TI? OR TITANIUM?)
L4             12 S L3 AND (GAS PHAS?)

=>

---Logging off of STN---



=>
Executing the logoff script...


=> LOG Y

STN INTERNATIONAL LOGOFF AT 11:33:20 ON 11 JUN 2007
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